

7. THE HEAVY GAS DISPERSION MODEL HEGADAS

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7. THE HEAVY GAS DISPERSION MODEL HEGADAS

In this chapter a technical description of the HGSYSTEM heavy gas dispersion model HEGADAS is given. As a reference description, in Chapter 7.A detailed technical information is given about the HEGADAS version (HEGADAS 5) which was available in HGSYSTEM version 1.0. This description still applies to the HEGADAS model as available in HGSYSTEM 3.0, apart from the changes that are described in Chapter 7.B and 7.C.

7.A. TECHNICAL DESCRIPTION OF THE HEGADAS MODEL

7.A.1. Introduction

Considerable quantities of flammable and toxic gases are produced, stored or transported throughout the world. Many of these gases are denser than air if released to the atmosphere. The gas may be heavier than air for several reasons; for example, because of high molecular weight (e.g. carbon dioxide CO₂), low temperature (e.g. liquefied natural gas, LNG), chemical transformations (e.g. polymerisation of hydrogen fluoride, HF), or the formation of liquid aerosols.

Safety considerations necessitate the assessment of the hazards that might ensue in the event of an accidental gas release. Such an assessment involves the study of the gas-dispersion processes, and should lead to an estimate of (or upper bound for) the gas concentration as a function of position relative to the source and time.

Among the most well-known large-scale tests are the Thorney Island field tests (McQuaid, 1984), the Burro field tests (Koopman et al., 1982), the Maplin field tests (Puttock, Colenbrander and Blackmore, 1984), and the Goldfish field tests (Blewitt, 1988).

A large number of heavy-gas dispersion models exist for predicting the dispersion of dense gas clouds; see, for example, Hanna and Drivas (1987) and Witlox (1991) for a review of vapour-cloud-dispersion models. Most heavy-gas-dispersion models are based on empirical similarity profiles for the concentration. These profiles are usually expressed in terms of the centre-line ground-level concentration, and vertical/cross-wind dispersion parameters. The latter quantities are determined from a number of basic equations describing gas-mass conservation, air-entrainment, cross-wind gravity spreading and cross-wind diffusion. Most models include a thermodynamical description, which assumes that the heavy gas is an ideal, non-reactive gas.

The Shell program HEGADAS ('HEavy GAs Dispersion from Area Sources) is a well developed and validated heavy gas dispersion similarity model. HEGADAS is a further improvement of a mathematical model developed by Te Riele (1977) for the prediction of gas concentrations in ground-level plumes emitted by area sources in steady-state situations. HEGADAS was originally developed by Colenbrander (1980, 1984) for both steady-state and transient releases. Colenbrander and Bond (1986) included the effects of heat and water vapour transfer from the substrate. This version of HEGADAS (called HEGADAS-4) is documented by Colenbrander and Puttock (1988) and Witlox (1988).

HEGADAS can be used both for steady-state calculations (using the HEGADAS-S version of the model) or for transient (time-dependent) calculations (using the HEGADAS-T model).

Chapter 7.A contains a detailed technical description of the version HEGADAS-5 of HEGADAS as it was available in HGSYSTEM version 1.0, and includes a large number of enhancements and extensions compared to HEGADAS-4. The description in Chapter 7.A serves as a reference point in the technical specification of HEGADAS-5. The HEGADAS version which is available in HGSYSTEM 3.0 is almost identical to HEGADAS-5. The main differences between HEGADAS-5 and the HGSYSTEM 3.0 version of HEGADAS are described in Chapter 7.B and 7.C.

HEGADAS-5 has in part been developed in a multi-sponsored project to produce a software package (HGSYSTEM) for modelling the release/dispersion of hydrogen fluoride (HF) and ideal gases. This project has been documented by the HGSYSTEM version 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) and the HGSYSTEM version 1.0 Program User's Manual (Witlox, McFarlane, Rees and Puttock, 1990). The latter documentation includes historical details not contained in Chapter 7 of this Manual.

The steady-state HEGADAS-5 model is also described in Witlox (1994a) and the transient model in Witlox (1994b). The interfacing of different HGSYSTEM modules is also discussed in Witlox and McFarlane (1994).

The two thermodynamical models available in the HGSYSTEM 3.0 HEGADAS model are described in full detail in Chapter 2.

The plan of this Chapter is as follows.

Section 7.A.2 describes the basic similarity model for *steady-state dispersion*. This model includes a new cross-wind gravity-spreading formulation, which accounts for the phenomenon of collapse of gravitational spreading, and a generalised cross-wind diffusion law for improved prediction of cross-wind diffusion far downwind (e.g. possible use of Briggs formula for cross-wind dispersion coefficient σ_y).

Section 7.A.3 describes the *time-dependent model* for dispersion downwind from either a horizontal ground-level source or a vertical transition plane with a near-field model.

Section 7.A.3.2 describes the new algorithm with which the concentrations are determined as a function of time and downwind distance.

Section 7.A.3.3 includes a new formulation which describes the spreading and evaporation of a horizontal ground-level pool (gas-blanket formulation).

Section 7.A.3.4 contains a new formulation with time-dependent dispersion calculations being started from a vertical transition plane (breakpoint); thus the heavy gas dispersion model can be interfaced with near-source jet/plume models in the case of time-dependent pressurised releases.

Section 7.A.3.5 contains an improved formulation which describes the inclusion of along-wind-diffusion effects for transient releases.

Section 7.A.4 describes the interfacing of the heavy gas dispersion model with pool evaporation models and near-source jet/plume models.

In HGSYSTEM version 3.0, the heavy gas dispersion model HEGADAS can be interfaced with the pool-evaporation model LPOOL and with the near-source jet/plume models AEROPLUME and HFPLUME.

Section 7.A.5 describes the validation of the HEGADAS model.

Section 7.A.6 summarises the major conclusions of Chapter 7.A.

7.A.2. Steady-state model

The HEGADAS-5 steady-state model is also described in Witlox (1994a).

7.A.2.1. Wind-speed and concentration similarity profiles

The HEGADAS model adopts a power-law fit of the ambient wind speed for the velocity u

$$u = u_0 \left[\frac{z}{z_0} \right]^\alpha \quad (2.1)$$

where z is the height and z_0 is a reference height at which the velocity is u_0 . The exponent α is found by matching the power law against the atmospheric wind profile $u_a(z)$.

See Appendix 7.A.A for details of this matching and an expression for $u_a(z)$ in terms of the Von Kármán constant $\kappa = 0.41$, the ambient friction velocity u_* , the surface roughness z_R and the Monin-Obukhov length λ .

The HEGADAS model adopts a similarity profile for the concentration c (kg/m^3),

$$c(x, y, z) = c_A(x) \cdot \exp\left[-\left[\frac{z}{S_z(x)}\right]^\beta\right] \quad |y| < b$$

$$c(x, y, z) = c_A(x) \cdot \exp\left[-\left[\frac{|y| - b(x)}{S_y(x)}\right]^2 - \left[\frac{z}{S_z(x)}\right]^\beta\right] \quad |y| > b$$

(2.2)

In the above formula x , y and z are Cartesian co-ordinates with the x -, y - and z - directions corresponding to the downwind, crosswind and vertical directions, respectively.

The release of the gas is at a rectangular ground-level area source located at $-\frac{1}{2}L < x < \frac{1}{2}L$, $-B < y < B$, $z = 0$, with L being the source length and B the source half-width.

The parameter β in the concentration profile is at present taken to be $\beta = 1 + \alpha$.

Figure 7.A.1 illustrates the concentration profile (2.2), which is expressed in terms of the peak concentration c_A , the dispersion coefficients S_z , S_y and the half-width b .

7.A.2.2. Dispersion variables and effective cloud data

DISPERSION VARIABLES

The dispersion variables c_A , S_z , S_y , b in the concentration profile (2.2) need to be determined in order to evaluate the concentration as a function of downwind distance x , crosswind distance y and height z .

The amount of heat and water-vapour added to the cloud needs also be evaluated if heat and water-vapour transfer from the substrate is included.

Thus the following dispersion variables need to be calculated as a function of downwind distance.

1. the centre-line ground-level concentration c_A (kg of dry pollutant/ m^3)
2. the vertical dispersion coefficient S_z (m) defining the decay of the concentration in the vertical direction
3. the crosswind dispersion coefficient S_y (m) defining the decay of the concentration along the Gaussian flanks of the crosswind concentration profile

4. the half-width b (m) of the middle part of the crosswind profile (along which the ground-level concentration equals c_A), as S_y increases, b eventually becomes zero and the crosswind profile is purely Gaussian.
5. the heat H_e added from the surface (Joule/kmole of mixture)
6. the water-vapour y_{w3} added from the surface (kmole/kmole of mixture)

Instead of the centre-line ground-level concentration c_A (kg of dry pollutant/m³), HEGADAS also utilises as an alternative variable the centre-line ground-level molar pollutant fraction y_{pol} ; c_A is related to y_{pol} by

$$c_A = m_{dp} \cdot (1 - \eta_w) \cdot y_{pol} / V_m \quad (2.3)$$

where η_w is the mole fraction of water in the pollutant, m_{dp} the molecular weight of the dry pollutant (kg/kmole), and V_m the mixture volume at centre-line and ground level (m³/kmole).

For given values of y_{pol} and H_e , the thermodynamic model as described in Chapter 2, determines the thermodynamic data V_m , ρ_m , T_m , which are the volume, the density and the temperature of the mixture at centre-line and ground level.

EFFECTIVE CLOUD CHARACTERISTICS

In HEGADAS the equations for the above dispersion variables are expressed in terms of so called 'effective' characteristics of the cloud. At each downwind position x the gas cloud in HEGADAS is characterised by an effective cloud half-width B_{eff} , an effective cloud height H_{eff} , an effective cloud speed u_{eff} , an effective molar cloud flow M_{eff}^{mol} (kmole of mixture passing per second through vertical plane at downwind distance x), a uniform concentration chosen to be equal to c_A , and a uniform molar mixture volume chosen to be equal to V_m (m³/kmole).

The effective cloud characteristics B_{eff} , H_{eff} , u_{eff} , M_{eff}^{mol} can be expressed as functions of S_z , b and S_y by

$$B_{eff} = \frac{1}{c(x, 0, z)} \int_0^{\infty} c(x, y, z) dy = b + \frac{1}{2} \sqrt{\pi} S_y \quad (2.4)$$

$$H_{\text{eff}} = \frac{1}{c(x, y, 0)} \int_0^{\infty} c(x, y, z) dy = \frac{1}{\beta} \cdot \Gamma\left(\frac{1}{\beta}\right) \cdot S_z \quad (2.5)$$

$$\mathbf{u}_{\text{eff}} = \left[\int_0^{\infty} c dz \right]^{-1} \int_0^{\infty} \mathbf{u} \cdot c dz = \frac{\Gamma[(1+\alpha)/\beta]}{\Gamma[1/\beta]} \cdot \mathbf{u}_0 \cdot \left(\frac{S_z}{z_0}\right)^{\alpha} \quad (2.6)$$

$$\begin{aligned} M_{\text{eff}}^{\text{mol}} &= \frac{1}{V_m \cdot c_A} \int_0^{\infty} \int_{-\infty}^{\infty} \mathbf{u} \cdot c dz = \frac{2 \cdot u_0 \cdot \Gamma[(1+\alpha)/\beta]}{\beta \cdot z_0^{\alpha} \cdot V_m} \cdot (b + \frac{1}{2} \sqrt{\pi}) \cdot S_z^{1+\alpha} \\ &= 2 \cdot B_{\text{eff}} \cdot H_{\text{eff}} \cdot \mathbf{u}_{\text{eff}} / V_m \end{aligned} \quad (2.7)$$

7.A.2.3. Dispersion equations

The 6 unknown HEGADAS dispersion variables c_A , S_z , S_y , b , H_e , y_{w3} are determined from the following six equations.

1. A *continuity equation* describing the conservation of gas mass flowing through a plane $x = \text{constant}$,

$$\begin{aligned} E &= \int_0^{\infty} \int_{-\infty}^{\infty} \mathbf{u} \cdot c dz = \frac{2 \cdot u_0 \cdot \Gamma[(1+\alpha)/\beta]}{\beta \cdot z_0^{\alpha}} \cdot c_A \cdot (b + \frac{1}{2} \sqrt{\pi}) \cdot S_z^{1+\alpha} \\ &= c_A \cdot 2 \cdot B_{\text{eff}} \cdot H_{\text{eff}} \cdot \mathbf{u}_{\text{eff}} = (1 - \eta_w) \cdot m_{\text{dp}} \cdot y_{\text{pol}} \cdot M_{\text{eff}}^{\text{pol}} \end{aligned} \quad (2.8)$$

where E is the prescribed source strength (kg of dry pollutant released per second).

2. An empirical *entrainment law* describing the vertical entrainment of air into the top of the gas cloud (kmole/sec per unit of cloud width and per unit of cloud length) and substrate water-vapour transfer,

$$\frac{1}{2 \cdot B_{\text{eff}}} \cdot \frac{d}{dx} [M_{\text{eff}}^{\text{mol}}] = u_e (u_T) / V_0 + Q_{\text{wv}} \quad (2.9)$$

with $V_0 = 22.4 \text{ m}^3/\text{kmole}$ the molar volume of ideal gas at $0 \text{ }^\circ\text{C}$ and 1 atmosphere, u_e the vertical air-entrainment velocity and Q_{wv} the molar water-vapour flux from the surface.

In equation (2.9) it is assumed that dilution of the cloud is caused by vertical mixing at the top of the cloud, with the vertical entrainment velocity of air given by u_e . equation (2.9) states that the increase of molar cloud flow in the downwind direction equals the sum of

molar cloud entrainment of air through the top of the cloud (kmole/s/m²) and the molar water-vapour transfer from the substrate (kmole/s/m²).

The entrainment velocity u_e can be expressed in terms of an empirical entrainment function Φ ,

$$u_e(u_T) = \frac{\kappa \cdot u_T}{\Phi(Ri_*(u_T))} \quad (2.10)$$

with

$$\Phi(Ri_*) = \begin{cases} \frac{(1 + 0.8 \cdot Ri_*)^{1/2}}{(1 + \alpha)} & Ri_* > 0 \\ \frac{(1 - 0.6 \cdot Ri_*)^{-1/2}}{(1 + \alpha)} & Ri_* < 0 \end{cases}$$

and with the bulk Richardson number $Ri_*(u_T)$ defined by

$$Ri_*(u_T) = g \cdot \frac{(\rho_m - \rho_{amb}(z = H_{eff}))}{\rho_{amb}(z = 0)} \cdot \frac{H_{eff}}{u_T^2} \quad (2.11)$$

where g is the gravitational acceleration ($= 9.81 \text{ m/s}^2$), κ is the Von Kármán constant ($= 0.41$) and ρ_{amb} the density of the ambient air. See Appendix 7.A.A for the evaluation of ρ_{amb} as a function of the height z .

The velocity u_T equals the friction velocity u_* if substrate heat transfer is not taken into account. Otherwise it is a modification of the friction velocity u_* to account for air entrainment caused by convection as a result of the temperature difference between the substrate and a cold vapour cloud. See Appendix 7.A.C.3 for the evaluation of u_T .

Note that the Richardson number Ri_* is proportional to the density difference between the gas cloud and the air, and reduces to zero in the far-field, passive-dispersion region.

The function $\Phi(Ri_*)$ was determined empirically using experimental laboratory data. See Section 3 of Appendix 3 in the HGSYSTEM 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) for further historical details.

3. An empirical law describing the *gravitational spreading of the gas cloud* in the cross-wind direction. In this spreading law the following consecutive phases are distinguished:

- o The initial phase of gravity spreading is governed by a simple spreading law by Van Ulden (1984),

$$\frac{dB_{\text{eff}}}{dt} = C_E \cdot \sqrt{g \cdot H_{\text{eff}} \cdot \left[1 - \frac{\rho_{\text{amb}}(z=0)}{\rho_m} \right]} \quad (2.12a)$$

where $C_E = 1.15$ is the spreading constant. The above law expresses that a dense vapour plume will spread laterally due to the difference in density between itself and the surrounding air. There is no entrainment.

- o As a result of detailed comparisons between predictions of HEGADAS and an extensive set of wind-tunnel simulations of dense-gas plumes, it was found that the well-defined gravity-current head at the edge of such a plume can be destroyed by boundary-layer turbulence. Thus equation (2.12a) is only applicable up to the downwind position, at which *collapse of gravity spreading* takes place. This position was found to be well given by the position at which the following collapse criterion is first satisfied,

$$\frac{B_{\text{eff}} / H_{\text{eff}}}{\sqrt{Ri} \cdot \sqrt{1 + 0.8 \cdot Ri_*}} \geq \frac{8}{3 \cdot \kappa} \quad (2.12b)$$

with the Richardson number Ri given by

$$Ri = g \cdot \frac{(\rho_m - \rho_{\text{amb}}(z=0)) H_{\text{eff}}}{\rho_m u_*^2}$$

- o The considerably reduced post-collapse lateral spreading was found to be well defined by

$$\frac{dB_{\text{eff}}}{dx} = \frac{1}{u_{\text{eff}}} \cdot \frac{dB_{\text{eff}}}{dt} = \frac{u_*}{u_{\text{eff}}} \cdot \frac{Ri \cdot \sqrt{1 + 0.8 \cdot Ri_*}}{3 \cdot \kappa \cdot C_D} \cdot \frac{H_{\text{eff}}}{B_{\text{eff}}} \quad (2.12c)$$

where $C_D = 5$ is an empirical constant.

- o The gravity spreading is neglected downwind of the point at which the crosswind profile becomes purely Gaussian (i.e. at the point at which b reduces to 0). If the gas becomes buoyant ($Ri_* < 0$) in the region $b > 0$, zero gravity spreading ($B_{\text{eff}} = \text{constant}$) is assumed.

The gravity-spreading law has been formulated by Roberts, Puttock and Blewitt (1990). Figure 2 compares the old HEGADAS-4 and new HEGADAS-5 models with the HTAG

wind-tunnel experiments (Petersen and Ratcliff, 1989). Section 7.3.2 and Chapter 8 in the HGSYSTEM 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) include further details and experimental evidence for the gravity-spreading model.

4. The derivation of the differential equation for the *cross-wind dispersion coefficient* S_y is based on an empirical formula for the non-dense cross-wind dispersion coefficient σ_y .

In HEGADAS-4, this formula was restricted to a power-law dependence of σ_y on the downwind distance x . The steps in a generalised formulation for the evaluation of S_y are described in detail in Appendix 7.A.B and can be summarised as follows:

- A Gaussian cross-wind concentration profile $c = c_a \exp(-\frac{1}{2}(y / \sigma_y)^2)$ is considered with the non-dense cross-wind dispersion coefficient σ_y given as an empirical function $\sigma_y^e(x)$ of the downwind distance x . The inverse of this function is denoted by $x^e(\sigma_y)$.
- The 2D cross-wind diffusion equation $u_x \partial c / \partial x = \partial / \partial y (K_y \partial c / \partial y)$ is considered. The cross-wind diffusion coefficient K_y is assumed to be proportional to the wind speed $u(z)$, $K_y = k_y \cdot u$, with $k_y = k_y^e(W)$ a function of the cloud half-width $W = (\pi / 2)^{1/2} \cdot \sigma_y$.
- Insertion of the formulas for c and K_y into the diffusion equation can be shown to lead to $k_y^e(W) = \sigma_y \partial \sigma_y^e / \partial x [x = x^e(\sigma_y)]$ with $\sigma_y = (2 / \pi)^{1/2} \cdot W$.

The derivation of the above formula for k_y is based on a Gaussian cross-wind concentration profile. In the HEGADAS concentration profile (2.2) the cross-wind dispersion coefficient S_y corresponds to $2^{1/2} \cdot \sigma_y$; the concentration c is uniform in a middle part of half-width b and it exhibits Gaussian decay for $|y| > b$ only.

Instead of the cloud half-width $W = (\pi / 2)^{1/2} \cdot \sigma_y$, HEGADAS adopts the effective cloud half-width $B_{\text{eff}} = b + \frac{1}{2} \cdot \pi^{1/2} \cdot S_y$. Therefore, in the calculation of S_y in HEGADAS-5 the following generalised equation is adopted to describe passive diffusion in the crosswind direction,

$$S_y \frac{\partial S_y}{\partial x} = 2 \cdot k_y^e(B_{\text{eff}}) \quad (b > 0) \quad (2.13)$$

Downwind of the position x_t at which b reduces to zero, S_y is taken to be defined by

$$S_y(x) = 2^{1/2} \cdot \sigma_y^e(x + x_v) \quad (b = 0) \quad (2.13^*)$$

with x_v chosen such that S_y is continuous at x_t .

In HEGADAS equations (2.13) and (2.13*) are applied to the empirical formula $\sigma_y^e(x) = \delta \cdot x \cdot (1 + \gamma \cdot x)^{-1/2}$ recommended by Briggs (1973). In this formula $\gamma = 0.0001 \text{ m}^{-1}$ and δ is related to the averaging time t_{av} (seconds) by $\delta = \delta_{600} \cdot (t_{av}/600)$ with $\delta_{600} = 0.22, 0.16, 0.11, 0.08, 0.06, 0.04 \text{ m}^{-1}$ for stability classes A, B, C, D, E and F, respectively.

5. The *heat transfer* equation

$$\frac{1}{2 \cdot B_{eff}} \cdot \frac{d}{dx} [H_e \cdot M_{eff}^{mol}] = Q_H \quad (2.14)$$

describes the heat flux Q_H transferred from the substrate to the gas cloud (Joule/sec per unit of cloud width and per unit of cloud length). The term between brackets in equation (2.14) represents the cloud heat flow through the plane $x = \text{constant}$, caused by pick-up of heat from the substrate (Joule/sec).

HEGADAS takes into account both free and forced heat convection. See Appendix 7.A.C.1 for full details of the evaluation of the heat flux Q_H .

6. The *water-vapour transfer* equation

$$\frac{1}{2 \cdot B_{eff}} \cdot \frac{d}{dx} [y_{w3} \cdot M_{eff}^{mol}] = Q_{wv} \quad (2.15)$$

describes the water-vapour flux Q_{wv} transferred from the substrate to the gas cloud (kmole/sec per unit of cloud width and per unit of cloud length). The term between brackets in equation (2.15) represents the molar flow of water through the plane $x = \text{constant}$, caused by pick-up of water-vapour from the substrate (kmole/sec). See Appendix 7.A.C.2 for full details of the evaluation of the water-vapour flux Q_{wv} .

7.A.2.4. Solution to dispersion equations

The entrainment law (2.9), the cross-wind gravity-spreading equation (2.12a) or (2.12b), the cross-wind diffusion equation (2.13), the heat-transfer equation (2.14) and the water-vapour transfer equation (2.15) provide *five ordinary differential equations*.

In HEGADAS these differential equations are solved in terms of the basic solution variables, which are chosen to be the effective molar cloud flow M_{eff}^{mol} , the effective cloud half-width B_{eff} , the cross-wind dispersion coefficient S_y , the added heat H_e from the surface, and the mole fraction y_{w3} of water-vapour added from the surface. The right-hand side of the differential equations is evaluated as follows as a function of these basic variables:

- y_{pol} is set from $M_{\text{eff}}^{\text{mol}}$ by applying the dry-pollutant conservation equation (2.8),
- V_m, ρ_m, T_m are set from y_{pol}, H_e using the relevant thermodynamic model (see Chapter 2); c_A is set from (2.3),
- S_z, H_{eff} are set from equations (2.8) and (2.5), b is found from (2.4)
- Q_H is set from equations (C.2), (C.4) and (C.7) and Q_{wv} from equation (C.10).

DISPERSION CALCULATIONS FROM GROUND-LEVEL POOL

For a ground-level pool (unpressurised release) the dispersion calculations are carried out as follows:

1. In HEGADAS-S the user-prescribed, so-called '*primary*' gas source, is assumed to be rectangular with specified length L_p (m), half-width B_p (m) and source strength E (kg of dry pollutant released per second).

Above the pool HEGADAS assumes a uniform centre-line ground-level concentration c_A , zero cross-wind gravity-spreading ($B_{\text{eff}} = \text{constant}$), zero cross-wind diffusion ($S_y = 0$) and zero heat and water-vapour transfer from the substrate ($H_e = y_{w3} = Q_H = Q_{\text{wv}} = 0, u_T = u_*$).

For given source dimensions L_p, B_p the maximum amount of dry pollutant that can be taken up by the atmosphere is found from equation (2.8) to be

$$E_{\text{max}}(B_p, L_p) = (1 - \eta_w) \cdot m_{\text{dp}} \cdot M_{\text{eff}}^{\text{mol}}(x = \frac{1}{2}L_p) \quad (2.16)$$

The following two cases are now distinguished:

- o If the specified source rate E is larger than the maximum take-up rate $E_{\text{max}}(B_p, L_p)$, all pollutant *cannot* be taken up directly by the atmosphere and a so-called 100 % *gas blanket or secondary pool* is assumed to form.

The blanket dimensions B, L are chosen in such a way that the aspect ratio stays the same, $B/L = B_p/L_p$, and such that $E = E_{\text{max}}(B, L)$ is satisfied. To this purpose equation (2.9) is solved iteratively with different start values of L ; $B = (B_p/L_p) \cdot L$ until equation (2.8) is satisfied at the downwind edge ($x = \frac{1}{2}L$) of the secondary pool.

- o If $E < E_{\max}(B_p, L_p)$ all released pollutant can be taken up directly by the atmosphere, a 100 % gas blanket *does not* form and the secondary pool equals the primary pool: $L = L_p, B = B_p$.

The mole fraction y_{pol} above the pool is less than one and is determined by solving equation (2.9) iteratively with different start values of y_{pol} until equation (2.8) is satisfied at the downwind edge ($x = 1/2L$) of the pool.

After y_{pol}, B and L have been determined as described above, the dispersion variables are calculated above the secondary pool ($-1/2L < x < 1/2L$):

- $B_{\text{eff}} = B, S_y = H_e = y_{w3} = 0,$
- V_m, ρ_m, T_m are set from y_{pol}, H_e using the relevant thermodynamic model,
- S_z is determined by solving the entrainment law (2.9) with $Q_{\text{wv}} = 0, u_T = u_s.$

2. The dispersion calculations downwind of the pool are carried out starting from the initial conditions at the downwind edge ($x = 1/2L$) of the pool. The entrainment law (2.9), crosswind gravity-spreading equation (2.12a) or (2.12b), crosswind diffusion equation (2.13), and the heat and water-vapour transfer equations (2.14), (2.15) are solved stepping forward in the downwind distance x .

After b has reduced to 0, the crosswind spreading and diffusion equations (2.12a) or (2.12b), (2.13) are no longer solved and S_y is set from equation (2.13*).

The variables S_z, H_e, y_{w3} are calculated from the differential equations (2.9), (2.14) and (2.15) with B_{eff} taken to be constant and $M_{\text{eff}}^{\text{mol}} = 2 \cdot B_{\text{eff}} \cdot H_{\text{eff}} \cdot u_{\text{eff}} / V_m,$

$$\frac{d}{dx} [H_{\text{eff}} \cdot u_{\text{eff}} / V_m] = u_e (u_T) / V_0 + Q_{\text{wv}} \quad (2.9^*)$$

$$\frac{d}{dx} [H_e \cdot H_{\text{eff}} \cdot u_{\text{eff}} / V_m] = Q_H \quad (2.14^*)$$

$$\frac{d}{dx} [y_{w3} \cdot H_{\text{eff}} \cdot u_{\text{eff}} / V_m] = Q_{\text{wv}} \quad (2.15^*)$$

Please note that the algorithm for $b = 0$ *has been changed* in the HEGADAS version as available in HGSYSTEM version 3.0. See Chapter 7.B. for a description of this new algorithm.

DISPERSION CALCULATIONS FROM TRANSITION POINT

For a pressurised release the momentum-dominated flow in the near field cannot be calculated by HEGADAS. Hence initial values of the dispersion variables at an appropriate transition point must be provided. Section 7.A.4.2 details how these data can be provided by a near-field model (e.g. HFPLUME or PLUME (HGSYSTEM 1.0) or AEROPLUME (HGSYSTEM 3.0)). Starting from these initial conditions the dispersion calculations are carried out as described in the above point 2.

PASSIVE LIMIT IN FAR FIELD

Both the entrainment law (for Richardson number $Ri_* \rightarrow 0$) and the crosswind spreading formulation (after b has reduced to 0) converge to the *passive-dispersion* limit in the far field. Moreover, the concentration profile becomes purely Gaussian after b has reduced to 0. Thus the HEGADAS formulation gives similar results to conventional passive-dispersion Gaussian models in the far field. The various phases in the dispersion of a steady ground-level release of propane (boiling liquid pool) are indicated in Figure 3.

SOLUTION OF DISPERSION EQUATIONS FOR HF; EQUIVALENT MOLES

When using the hydrogen fluoride chemistry and thermodynamics as described in Chapter 2.B, y_{pol} , H_e , y_{w3} and M_{eff}^{mol} are assumed to be associated with *equivalent moles* of mixture based on *all* HF being in the monomer state, and equations (2.7), (2.9), (2.9*), (2.14), (2.14*), (2.15), (2.15*) refer to equivalent moles. [Note that strictly speaking for equation (2.3) to be correct V_m should be the volume of the pollutant per equivalent mole and not volume of the pollutant per 'real' mole!].

7.A.3. Time-dependent model

The HEGADAS-5 transient model HEGADAS-T is also described in Witlox (1994b).

7.A.3.1. Introduction

The time-dependent (or transient) version HEGADAS-T of HEGADAS-5 can be used to model the time-dependent ground-level dispersion of a heavy gas cloud which moves with the ambient wind.

It can be used to model the dispersion downwind of either a time-dependent ground-level source (unpressurised release) or a vertical transition plane (or breakpoint; pressurised

release). The dispersion variables at the transition plane are determined from a near-source jet/plume program (see Sections 7.A.4.2 and 7.A.4.3).

In HEGADAS-T the transient behaviour of the dense vapour cloud is approximated by a quasi-steady-state description in which so-called '*observers*' are released at the pool/transition-plane at a series of times. These observers travel with the wind. The concentration data are determined as a function of position and time by means of the following algorithmic steps.

1. For a ground-level source, the time-dependent pool dimensions and pool evaporation rate (primary pool) are user-specified or are provided from pool evaporation models (see Section 7.A.4.1). If the pool emission rate becomes larger than the maximum amount of gas which can be taken up by the air, a gas blanket forms (secondary pool). Observers are 'released' at a series of times upwind of the gas blanket. *These observers travel with the wind.* The blanket data observed by each observer are determined.

For a vertical-plane transition from a near-source jet model, the values of the HEGADAS dispersion variables at the transition plane are determined by means of matching against the values of the dispersion variables for the jet model. The observers are released at the transition plane (breakpoint).

2. For each observer, the observed concentration is computed via steady-state HEGADAS calculations adopting the observed source data. Thus, by calculating the position of each observer at a given time t , the concentrations are determined at time t for a number of downwind distances from the pool/breakpoint.
3. A cloud shape correction is applied to the observer concentrations. This correction introduces downwind gravity spreading and reduces the calculated cross-wind gravity spreading in such a way that the amount of spreading in the downwind direction of the cloud as a whole equals the spreading in the cross-wind direction.
4. At a given time t , the actual concentration is determined from Gaussian integration with respect to the downwind distance x of the above observer concentrations. This Gaussian integration involves a downwind dispersion coefficient σ_x , which allows longitudinal diffusion to be taken into account.

Section 7.A.3.2 describes in more detail the new algorithm with which the concentrations are determined.

Sections 7.A.3.4.3 and 7.A.3.4.4 describe the models for a ground-level pool and a vertical transition plane, respectively.

Section 7.A.3.4.5 describes the along-wind-diffusion formulations adopted in the model.

See Appendix 7.A.E for the evaluation of the observer position as a function of time and see Appendix 7.A.F for details on the cloud shape correction.

7.A.3.2. Algorithm for evaluation of concentrations

In HEGADAS-4 the user had to specify the time interval Δt_{obs} with which observers were to be released. This procedure required the user to be familiar with the observer concept, since selection of too large a time step leads to inaccurate concentration predictions at the specified output times. This section describes the algorithm for evaluation of concentrations in HEGADAS-5 (as available in HGSYSTEM version 1.0).

In this algorithm Δt_{obs} is determined internally in the program to ensure accurate predictions (automated release of observers).

For a horizontal ground-level source, observers are released with a constant time interval Δt_{obs} at the upwind edge of the source. The observers travel with the wind in the downwind direction. While travelling over the time-varying source, each observer i ($i = 1, 2, \dots, M$) 'sees' a source length L_i (m; in downwind direction), an averaged source half-width B_i (m; in cross-wind direction), a source strength E_i (kg/s) and a downwind edge of the source x_{dw}^i (m); see Section 7.A.3.3 for the evaluation of the observer source data.

Steady-state dispersion calculations based on these data yield the observer-dispersion data: ground-level centre-line wet-pollutant molar fraction $y_{\text{pol}}^i(x) = y_{\text{pol}}(x - x_{\text{dw}}^i + L_i/2; E_i, B_i, L_i)$, vertical dispersion coefficient $S_z^i(x) = S_z(x - x_{\text{dw}}^i + L_i/2; E_i, B_i, L_i)$, etc.

Here for example $y_{\text{pol}}(x; E, B, L)$ corresponds to a steady-state ground-level source with strength E , half-width B , length L and source centroid at $x = y = 0$.

For a vertical transition plane (breakpoint), observers $i = 1, 2, \dots, M$ are released with a constant time interval Δt_{obs} at the breakpoint. For each observer i , steady-state dispersion calculations are carried out based on the breakpoint data valid at the time the observer is released.

Let x_j^i be the position of observer i at the output time t_j ($j = 1, 2, \dots, N; t_1 < t_2 < \dots < t_N$).

Then $x_j^1 > x_j^2 > \dots > x_j^M$, i.e. *observers released earlier are located further downwind*.

The concentration data $y_{\text{pol}}(x, t_j)$, as a function of the downwind distance x at the output time t_j , are derived from the observer-dispersion data $c_j^i = y_{\text{pol}}^i(x_j^i)$, $i = 1, 2, \dots, N$ by the inclusion of a

cloud-shape correction for gravitational spreading and the inclusion of downwind diffusion effects. Thus for an accurate evaluation of $y_{\text{pol}}(x,t)$, the release interval Δt_{obs} (determining the observer spacing) must be smaller if larger gradients of $y_{\text{pol}}(x,t)$ occur.

The observer concept in HEGADAS-T is a *quasi-steady-state solution method* for determining the concentration $y_{\text{pol}}(x,t)$ as a function of the downwind distance x and the time t . This method may be seen as a *first-order inclusion of time-dependent effects*. It produces accurate predictions for slowly varying time-dependent sources, but it may lead to less accurate predictions for rapidly time-varying sources.

CRITERION FOR CHOOSING NUMBER OF RELEASED OBSERVERS

In a HEGADAS-T run the concentrations calculated at each output time t_j must be accurate. This condition requires a sufficiently small spacing of the observers, i.e. a sufficiently small value of the observer-release interval Δt_{obs} such that the concentration curve $y_{\text{pol}}(x,t_j)$ can be evaluated accurately from the observer-dispersion data.

An observer spacing that is too large leads to concentration curves that are *too smooth* (peaks are eroded).

Consider the positions $x_j^{i+1}, x_j^i, x_j^{i-1}$ ($x_j^{i+1} < x_j^i < x_j^{i-1}$) and the concentrations $c_j^{i+1}, c_j^i, c_j^{i-1}$ seen by three adjacent observers $i+1, i, i-1$ ($i = 2, \dots, M-1$).

Let C_j^i be the estimate of the concentration at x_j^i based on linear interpolation of the data for observers $i+1$ and $i-1$ (*before* the inclusion of the cloud-shape correction and downwind-diffusion effects).

C_j^i thus equals

$$C_j^i = c_j^{i+1} + (x_j^i - x_j^{i+1}) \cdot \left(\frac{c_j^{i-1} - c_j^{i+1}}{x_j^{i-1} - x_j^{i+1}} \right) \quad (3.1)$$

This would have been the HEGADAS estimate of the concentration at x_j^i , if observer i would not have been released.

Thus the estimates of the absolute error $\epsilon_j^{\text{abs},i}$ and relative error $\epsilon_j^{\text{rel},i}$ at x_j^i are

$$\begin{aligned} \epsilon_j^{\text{abs},i} &= |C_j^i - c_j^i| \\ \epsilon_j^{\text{rel},i} &= |C_j^i - c_j^i| / c_j^i \end{aligned} \quad (3.2)$$

A convergence criterion for the observer concentrations must be chosen carefully. For smaller output times, the gas cloud may have very 'sharp' edges. The relative and absolute concentration errors near these edges will only be small for a very large number of observers and an excessive amount of computer time.

Hence, instead of demanding that the maximum value of the concentration error is small, it is more appropriate to demand that the *mean* concentration error is small. Effectively this means that the *predicted cloud volume* or *cloud shape* is accurately modelled.

The *peak* concentrations must be accurately predicted. Thus at each output time, error estimates for observers with larger concentrations should contribute more than those with minute concentrations. Hence it is more appropriate to demand small mean *absolute* concentration errors than small mean relative concentration errors.

The relative error in the predicted cloud volume or cloud shape must be small for every output time. Hence it is appropriate to scale the mean absolute concentration error at a given output time with the peak concentration at that time. Thus the following convergence criterion for the observer concentrations is adopted

$$\max_{1 \leq j \leq N} \left[\frac{1}{M-2} \cdot \frac{\sum_{i=2}^{M-1} \epsilon_j^{\text{abs},i}}{\max_{1 \leq i \leq M} c_j^i} \right] < \epsilon_{\text{obs}} \quad (3.3)$$

The above convergence criterion implies that for all times t_j ($j = 1, 2, \dots, N$), the ratio of the mean error in the absolute concentration and in the peak concentration is smaller than the convergence tolerance ϵ_{obs} .

The default value of ϵ_{obs} adopted in HEGADAS-T equals $\epsilon_{\text{obs}} = 0.05$. This value was found to lead to accurate concentration predictions without an excessive number of observers for most types of source conditions. [It is noted that the averaging of the concentration in the numerator of equation (3.3) is only applied to those observers which actually have seen (some part of) the source at time t_j .]

CRITERION FOR CHOICE OF OUTPUT TIMES

The maximum concentration over all times, $c_{\text{max}}(x)$ must normally be determined accurately. This condition requires a sufficiently close spacing between the output times t_1, t_2, \dots, t_N , such that the envelope $c_{\text{max}}(x)$ of the curves $c(x, t_1), c(x, t_2), \dots, c(x, t_N)$ is well defined.

The user can verify that this condition is satisfied by plotting a series of these curves in one graph. The plot file corresponding to each curve $c(x,t_j)$ can be generated by the interactive HEGADAS-T post-processor HTPOST (HGSYSTEM version 1.0) or the batch post-processor POSTHT (HGSYSTEM 3.0). See the relevant information on POSTHT in the HGSYSTEM 3.0 User's Manual.

HEGADAS-T ALGORITHM WITH AUTOMATED RELEASE OF OBSERVERS

In HEGADAS the time-dependent pool or transition data are specified with a fixed time step Δt .

Let n_{td} be the number of records and t_{st} be the start time; for a ground-level pool t_{st} equals the time at which the pool becomes active, and for a transition plane it equals the time at which pollutant first passes the transition plane.

Thus the data are specified at the input times $t_{st}+\Delta t$, $t_{st}+2\cdot\Delta t$, ..., $t_{st}+n_{td}\cdot\Delta t$. Zero data are assumed for time $t > t_{st}+(n_{td}+1)\cdot\Delta t$.

Data are linearly interpolated between the input times.

The automation of the release of observers in HEGADAS-T is carried out by means of the following consecutive algorithmic steps:

1. For a ground-level source the primary-pool data and secondary-pool (gas-blanket) data are set as a function of time (see Section 7.A.3.3.1).

The maximum blanket radius R_{max} is determined.

The observers are released at $x = -R_{max}$. The minimum and maximum observer-start times for which an observer may see a pool (t_{min}^{st} , t_{max}^{st}) are determined.

Observer-source data (secondary source data seen by the observer while travelling over the pool) are set for the maximum number of (currently) 161 observers (see Section 7.A.3.3.2).

Observers 1, 2, ..., 160, 161 are released at the times t_{min}^{st} , $t_{min}^{st}+\Delta t_{obs}$, ..., $t_{max}^{st}-\Delta t_{obs}$, t_{max}^{st} , with the observer-release interval given by $\Delta t_{obs} = (t_{max}^{st} - t_{min}^{st})/160$.

For a vertical transition plane, breakpoint data are set and observers are released at the times $t_{st}+\Delta t_{obs}$, $t_{st}+2\cdot\Delta t_{obs}$, ..., $t_{st}+161\cdot\Delta t_{obs}$, where $\Delta t_{obs} = (n_{td}+1)\cdot\Delta t/162$ (see Section 7.A.3.4).

2. a The initial observer release interval is currently chosen to be equal to $IFREQ = 32$, and dispersion data are set for the 6 observers 1, 33, 65, 97, 129, 161 (5 observer intervals).
 - b If the convergence criterion (3.3) is satisfied for the current observers 1, $1+IFREQ$, ..., $161-IFREQ$, 161 go to step 3.

c If IFREQ = 1, terminate program with an error message saying that convergence can not be obtained with the maximum number of 161 observers.

d Double the number of observer intervals, i.e. set dispersion data for the additional, intermediate observers $1+IFREQ/2$, $1+3\cdot IFREQ/2$, ..., $161-3\cdot IFREQ/2$, $161-IFREQ/2$, and half observer frequency ($IFREQ = IFREQ/2$). Go to step 2b.

3. Carry out cloud shape correction of dispersion data for observers 1, $1+IFREQ$, ..., $161-IFREQ$, 161 (see Appendix 7.A.F) and include downwind-diffusion effects (see Section 7.A.3.5).

7.A.3.3. Dispersion from ground-level source

7.A.3.3.1. Secondary source

For finite-duration steady-state releases or slowly varying release rates the HEGADAS-T (version HEGADAS-4) formulation lead to erroneous oscillatory behaviour in the predictions of the dimensions of the gas blanket (secondary source).

This section introduces an improved formulation without oscillatory behaviour. See Section 7.5 in the HGSYSTEM 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) for further historical details.

In the model the primary source is assumed to be circular with a radius $R_p(t)$, m, and a dry-pollutant emission rate $E(t)$, kg/s.

A 100 % vapour blanket is assumed to form if $E(t)$ is larger than the maximum take-up rate $E_{\max}[B=1/2\pi^{1/2}\cdot R_p(t), L=\pi^{1/2}\cdot R_p(t)]$ corresponding to an equivalent steady square pool that has the same area $\pi\cdot R_p^2(t)$ as the circular source (see equation (2.16)).

The gas blanket is taken to have a flat cylindrical shape of radius $R_g(t)$ and height $H_g(t)$. The blanket dimensions $R_g(t)$ and $H_g(t)$ are determined from the numerical solution of two differential equations representing a gravity-spreading law [analogous to the spreading equation (2.12a)] and blanket-mass conservation, respectively,

$$\frac{dR_g(t)}{dt} = C_E \cdot \sqrt{g \cdot \frac{\rho_E - \rho_a(z=0)}{\rho_E}} \cdot H_g(t) \quad (3.4)$$

$$\frac{dM(t)}{dt} = E(t) - E_{\max} \cdot [B = 1/2 \pi^{1/2} \cdot R_g(t), L = \pi^{1/2} \cdot R_g(t)] \quad (3.5)$$

Here ρ_E is the dry-pollutant density, kg/m^3 , $g = 9.81 \text{ m/s}^2$ the acceleration of gravity and $M(t)$ the blanket mass defined by

$$M(t) = \pi \cdot \rho_E \cdot R_g^2(t) \cdot H_g(t) \quad (3.6)$$

At the onset of the formation of the gas blanket, say at time $t = t_0$, the blanket radius equals the primary source radius and the blanket mass equals zero. Thus in the numerical solution of equations (3.4), (3.5) the initial values $R_g(t_0) = R_p(t_0)$ and $M(t_0) = 0$ are adopted. The differential equations are subsequently solved stepping forward in time.

For $t > t_0$ the blanket radius $R_g(t)$ increases as a result of gravity spreading; see equation (3.4). Mass is added to the gas blanket because of material entering the pool [spill rate $E(t)$] and lost because of evaporation [evaporation rate $E_{\max}[B=1/2\pi^{1/2} \cdot R_p(t), L=\pi^{1/2} \cdot R_p(t)]$; see equation (3.5). Note that the amount of evaporation increases with the blanket radius $R_g(t)$.

For $t > t_0$ the blanket radius $R_g(t)$ is initially small and therefore the evaporation rate is less than the spill rate. Hence the mass of gas in the blanket initially increases. Because of this accumulation of gas, the blanket continues to spread beyond the radius at which the evaporation rate would equal the spill rate, and thereafter the evaporation exceeds the source rate. The mass of gas in the blanket therefore decreases, eventually reaching zero.

Let $t = t_1$ be the time at which the blanket height reduces to zero, i.e. the time at which the entire gas blanket is taken up into the air.

If the source rate $E(t_1)$ is smaller than $E_{\max}[B=1/2\pi^{1/2} \cdot R_p(t_1), L=\pi^{1/2} \cdot R_p(t_1)]$, the gas blanket disappears at time $t = t_1$ and the secondary pool is set equal to the primary pool.

If $E(t_1) > E_{\max}[B=1/2\pi^{1/2} \cdot R_p(t_1), L=\pi^{1/2} \cdot R_p(t_1)]$, a zero-height gas blanket forms. This gas blanket is assumed to equal the steady-state blanket corresponding to the present spillage rate $E(t_1)$. Thus according to equation (3.5) the pool radius $R_g(t_1)$ of this blanket is determined from inversion of the formula $E(t_1) = E_{\max}[B=1/2\pi^{1/2} \cdot R_p(t_1), L=\pi^{1/2} \cdot R_p(t_1)]$.

For $t > t_1$ a gas blanket with zero height is assumed to remain in existence as long as the gas-release rate does not increase [$dE(t)/dt < 0$] and the blanket radius exceeds the primary radius [$R_g(t) > R_p(t)$]. Let the end of this period be at time $t = t_2$. During the period $t_1 < t < t_2$ the blanket radius $R_g(t)$ is determined from the steady-state blanket corresponding to the release rate $E(t)$, i.e. it is determined from inversion of the formula $E(t) = E_{\max}[B=1/2\pi^{1/2} \cdot R_p(t), L=\pi^{1/2} \cdot R_p(t)]$.

At the end $t = t_2$ of the period the following two cases can be distinguished:

- The blanket radius $R_g(t)$ reduces to the primary radius $R_p(t)$ at $t = t_2$. In this case the zero-height gas blanket disappears and the secondary pool becomes equals to the primary pool.
- The release rate $E(t)$ starts to increase at time $t = t_2$. In this case a finite-thickness gas blanket forms and equations (4.4), (4.5) are solved with the initial values $R_g(t_2)$ (unchanged blanket radius) and $M(t_2) = 0$.

Summarising the above results the following applies for the radius $R(t)$ and the evaporation flux $Q(t)$, kg/m²/s of the secondary source:

$$\begin{aligned} R(t) &= R_g(t) && \text{(with gas blanket)} \\ R(t) &= R_p(t) && \text{(no gas blanket)} \end{aligned} \tag{3.7}$$

$$Q(t) = \frac{E_{\max} \cdot [B = \frac{1}{2} \pi^{\frac{1}{2}} \cdot R_g(t_1), L = \pi^{\frac{1}{2}} \cdot R_g(t_1)]}{[\pi \cdot R_g^2(t_1)]} \quad \text{(with gas blanket)}$$

$$Q(t) = \frac{E(t)}{[\pi \cdot R_p^2(t_1)]} \quad \text{(no gas blanket)}$$

The above formulation has been tested for a pool of boiling propane with a primary radius $R_p = 3$ m, a constant evaporation rate $E = 30.0$ kg/s and a release duration of 200 seconds. Figure 5 illustrates that the HEGADAS-5 model indeed eliminates the oscillatory gas-blanket behaviour of the former HEGADAS-4 model. Initially, a finite-thickness gas blanket forms. After this blanket has spread beyond the steady-state radius (≈ 15 m), the blanket mass diminishes until it is reduced to zero at time $t_1 \approx 25$ s. At this time the blanket radius is reset in the HEGADAS-5 model to the steady-state radius. In the HEGADAS-4 model the blanket radius is reset to the primary pool radius after each disappearance of the finite-thickness gas blanket.

7.A.3.3.2. Observer source data

The observers $i = 1, 2, \dots$ are released with a time interval Δt_{obs} upwind of the secondary pool, i.e. at $x = -R_{\text{max}}$, where R_{max} is the maximum blanket radius [= maximum value of $R(t)$].

The observers travel with the wind. Appendix 7.A.E describes the evaluation of the observer position $x^i(t)$ and observer speed $u^i(t)$ as a function of time. The observer velocity increases with downwind distance and for all observers their velocity at a given location x is the same ($u^i(x) = u^{i+1}(x)$).

This implies that at a given time t the velocity of observer i is greater than the velocity of the following observer $i+1$ ($u^i(t) > u^{i+1}(t)$).

Let us now consider one specific observer, say observer i , and let us follow this observer while it moves over the secondary pool. Let observer i encounter the upwind edge of the secondary source at $t = t_1^i$ and the downwind edge at $t = t_2^i$ and let $x^i(t)$ be the location of this observer at time t . As can be seen from Figure 6 the local secondary half-width of the source $B_{obs}^i(t)$ observed at time t is given by:

$$B_{obs}^i(t) = \sqrt{R^2(t) - (x^i(t))^2} \quad (3.8)$$

The secondary source area A^i and the source rate E^i seen by observer i is found by evaluating the integrals

$$A^i = \int_{t_1^i}^{t_2^i} 2 \cdot u^i(t) \cdot B_{obs}^i(t) dt \quad (3.9)$$

$$E^i = \int_{t_1^i}^{t_2^i} 2 \cdot Q(t) \cdot B_{obs}^i(t) \cdot u^i(t) dt \quad (3.10)$$

The secondary source length L^i as seen by observer i is given by:

$$L^i = x^i(t_2^i) - x^i(t_1^i) \quad (3.11)$$

and thus we find an averaged observed secondary half-width of the source

$$B^i = \frac{1}{2} \cdot A^i / L^i \quad (3.12)$$

In this way we can determine, for each of the n observers travelling over the source ($i = 1, \dots, n$), the observed dimensions L^i and B^i , the locations $x^i(t_1^i)$ and $x^i(t_2^i)$ of, respectively, the upwind and the downwind edge of the secondary source and the take-up rate E^i .

7.A.3.3.3. Concentrations

From the observer source data the concentration distribution in the cloud can be determined at a specified time t_s . To this end the location $x^i(t_s)$ of each observer at time t_s is calculated and for each observer a steady-state calculation is done, using the pertinent parameters L_i, B_i, E_i and $x^i(t_2^i)$. Thus the concentration distribution parameters $c_A(x^i(t_s)), S_y(x^i(t_s)), b(x^i(t_s)), S_z(x^i(t_s))$ are

determined for $i = 1, \dots, n$ and thus the concentration distribution $c(x^i(t_s), y, z)$ given by equation (2.2).

It will be clear that in this quasi-steady state approach the gravitational spreading of the cloud in the wind direction cannot be taken into account, unlike in heavy gas dispersion box models for strictly instantaneous vapour releases (e.g. HEGABOX).

Thus, the width of the cloud calculated with the model presented here will be somewhat too large and the length too small, especially at very low wind velocities.

Some spreading in the wind direction is introduced in the gas blanket calculation, where we can use a radial spreading law because the centre of the gas blanket is assumed to remain stationary above the source at $x = 0$.

In addition, a correction algorithm has been devised for use at the end of the calculation, which redistributes part of the lateral gravity spread to longitudinal spreading. Appendix 7.A.F includes a description of this *cloud shape correction*.

For releases of short duration, dispersion in the wind direction may have a significant influence on the concentration level in the cloud.

Accordingly, the calculated concentrations are adjusted to take account of this dispersion in the x-direction. The method followed is described in Section 7.A.3.5.

7.A.3.4. Dispersion downwind of transition with near-source jet model

7.A.3.4.1. Transition data

If HEGADAS-T is to be run downwind of a vertical transition plane $x = x_{br}$ (breakpoint) with a near-source jet model, three data are to be specified at the breakpoint by the user for a number of times.

These data are the effective cloud half-width $B_{eff}^{br}(t)$ and any two of the following breakpoint values: the ground-level centre-line wet-pollutant molar fraction $y_{eff}^{br}(t)$, the effective cloud height $V_{eff}^{br}(t)$, and the dry-pollutant mass flow $E^{br}(t)$ through the transition plane (kg/s).

Breakpoint data at other times are derived by linear interpolation.

It is assumed that at the breakpoint the cross-wind concentration profile is uniform and does not have Gaussian flanks [$b = B_{eff}^{br}(t)$, $S_y = 0$]. In addition, the amount of water-vapour y_{w3} and heat H_e added from the surface are taken to be zero [$y_{w3} = H_e = 0$]. From the specified breakpoint data described above, the dispersion variables y_{pol} and S_z at the breakpoint are then set using the equations described in Section 7.A.2.3.

7.A.3.4.2. Concentrations

The time-dependent values of the six dispersion variables y_{pol} (or c_A), S_z , b , S_y , H_e , y_{w3} determined at the breakpoint are used as starting values for the steady-state dispersion calculations for the observers, which are released with a fixed user-specified time interval Δt_{obs} . These calculations involve the solution of the dispersion equations described in Section 7.A.3.2. Thus, for each observer, dispersion data are obtained as a function of the downwind distance x .

In order to express the observer dispersion data as a function of position and time, a formula needs to be provided for the position of each observer as a function of time. See Appendix 7.A.A for a derivation of this formula. By use of this formula, the observer data are stored at those downwind positions, which correspond to a number of user-specified output times.

Appendix 7.A.B describes the subsequent application of the cloud shape correction for downwind gravity spreading to these data. After the cloud shape correction, downwind diffusion effects are taken into account as described in Section 7.A.4.

Note that the conditions at the breakpoint x_{br} remain satisfied during the inclusion of downwind diffusion. This is because zero diffusion ($\sigma_x = 0$) is assumed at $x = x_{\text{br}}$ in the along-wind-diffusion formulations.

EXAMPLES

First the problem is considered of a steady plume which starts to pass the transition plane at time $t = 0$. Figure 7 illustrates the HEGADAS-T predictions at time $t = 100$ seconds. As expected, the HEGADAS-T predictions at this time closely resemble the HEGADAS-S predictions for a corresponding steady release.

The formulation was also validated by a simulation of the first Goldfish experiment, in which the transition data were derived from the near-source jet/plume model HFPLUME.

Figure 8 shows that the time-dependent centre-line ground-level concentrations are predicted well by HEGADAS.

Chapter 9 in the HGSYSTEM version 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) includes full details.

7.A.3.5. Inclusion of along-wind-diffusion effects

The centre-line ground-level concentration $c_A = c_A(x,t)$ is calculated as a function of time t and distance x downwind of the source by means of *Gaussian integration of the observer concentrations* $C_A(\xi)$ at ξ ,

$$c_A(x, t) = \int_0^{\infty} \frac{C_A(\xi)}{\sqrt{2\pi} \cdot \sigma_x(\xi)} \cdot \exp\left[-\frac{(x-\xi)^2}{2\sigma_x^2(\xi)}\right] d\xi \quad (3.13)$$

In the above equation ξ is the position at time t of an observer travelling with the wind in the downwind direction. At this position the observer observes the concentration $C_A(\xi)$, where $C_A(\xi)$ is calculated from a steady-state HEGADAS solution based on zero along-wind diffusion (see Section 7.A.3.2).

In (3.13) along-wind diffusion is taken into account by assuming that the concentration $C_A(\xi)$ spreads out around ξ according to a Gaussian distribution with a downwind dispersion coefficient $\sigma_x = \sigma_x(\xi)$.

Note that the position ξ of the observer in equation (3.13) corresponds to the observer position *after* the cloud shape correction for gravitational spreading in the wind direction has been applied (see Appendix 7.A.F).

The dispersion coefficient σ_x is usually considered to consist of two statistically independent components σ_{xs} and σ_{xt} ,

$$\sigma_x = \sqrt{\sigma_{xs}^2 + \sigma_{xt}^2} \quad (3.14)$$

The component σ_{xs} is the spread induced by vertical wind shear and σ_{xt} is the turbulent spread caused by downwind-direction velocity fluctuations. Increasing the wind shear du/dz increases the relative speed at which the top and bottom of the cloud are advected, and so increased shear du/dz results in increased spread σ_{xs} . Since the wind shear increases with stability, the spread σ_{xs} increases with stability. This is confirmed by the experimental data of Nickola (1971).

LITERATURE REVIEW OF ALONG-WIND DIFFUSIONS FORMULATIONS

In the original HEGADAS-4 formulation the formula $\sigma_x = \sigma_x(\xi)$ did not take into account the change of wind shear and hence the formula was not altered as a function of the stability class.

The following provides an overview of along-wind-diffusion formulations in the literature.

1. Formula for σ_{xs} by Smith (passive flow).

Smith (1965) analysed the problem of shear diffusion of puffs released in the surface layer theoretically. Using the method of moments, he arrived at the following formula for σ_{xs} (source at ground level) valid for passive flow

$$\sigma_{xs} = \sigma_{xs}(\xi) = 12^{-1/2} \cdot \left(\frac{du}{dz} \right) \cdot t_{obs} \cdot \sigma_z \quad (3.15)$$

Here t_{obs} is the travel time of the puff from (the middle part of) the pool to the present puff position $x = \xi$, σ_z the vertical dispersion coefficient, and du/dz the vertical gradient of the horizontal wind speed $u(z)$ at a certain reference height (see e.g. point 3 below).

2. Formula for σ_{xs} by Chatwin (neutrally stratified, passive flow).

Chatwin (1968) studied the passive dispersion of a puff in a neutral atmosphere. He arrived at the following formula for the downwind dispersion coefficient σ_{xs} ,

$$\sigma_{xs} = \sigma_{xs}(\xi) = 0.596 \cdot u_* \cdot t_{obs} / \kappa \quad (3.16)$$

Here $\kappa = 0.41$ is the Von Kármán constant and u_* the ambient friction velocity.

The derivation of equation (3.16) by Chatwin is based on a logarithmic formula for the ambient wind speed u valid for neutrally stratified flow only, and the linear formula $K_z = \kappa \cdot u_* \cdot z$ for the vertical diffusivity (or $u_e = u_*$ for entrainment velocity) valid for passive gases only. HEGADAS adopts the more general formula (A.1) in Appendix 7.A.A for the wind speed for stratified flow and the heavy gas, non-passive extension (2.10) of the formula for the entrainment velocity.

The analytical derivation of equation (3.16) by Chatwin consists of two parts. In the first part the velocity $d\xi/dt$ and position ξ of a puff (frozen puff, moving with the wind) as a function of the travel time t_{obs} are calculated (see equation (23) in Chatwin (1968)).

The extension of this calculation to stratified, heavy-gas flow can be done relatively easily. See Chaudry and Meroney (1972) for an extension of this calculation to stratified flow.

In the second part σ_{xs} is calculated by applying the Lagrangian similarity hypothesis valid for neutrally stratified flow. This calculation can easily be extended to neutral, heavy-gas flow with a constant Richardson number, and equation (3.16) can be shown to be still valid. However, it cannot be extended in a straightforward manner to the non-neutral case.

3. Formula for σ_{xs} and σ_{xt} by Ermak (stratified, passive flow).

The formulation of Ermak (1986) is a further development of an along-wind-diffusion formulation by Wilson (1981) for stratified, passive flow. By using a purely Gaussian profile for the concentration and a power-law for the ambient wind speed, he expresses the puff velocity $d\xi/dt$ as a function of the vertical spreading coefficient σ_z .

Using a stability-class dependent power-law fit of an empirical formula for $\sigma_z(\xi)$ recommended by Briggs (1973), he then expresses $t_{obs} = t_{obs}(\xi)$ as a function of ξ .

Following Wilson, Ermak evaluated (du/dz) in equation (3.15) at a reference height found from matching equations (3.15) and (3.16). Insertion of the expression $t_{obs} = t_{obs}(\xi)$ into equation (3.15) then leads to the evaluation of σ_{xs} as a function of ξ .

Assuming isotropic horizontal turbulent spread ($\sigma_{xt} = \sigma_{yt}$), Ermak determines σ_{xt} from a formula recommended by Briggs (1973).

Thus the following formulas are used by Ermak:

$$\sigma_{xs}(\xi) = \left\{ \frac{0.60 \cdot \sqrt{\pi} \cdot 0.34^\alpha}{(1 - \alpha \cdot d) \cdot \Gamma(\frac{1}{2} + \frac{1}{2}\alpha)} \right\} \cdot \xi$$

$$\sigma_{xt}(\xi) = \frac{a_y \cdot \xi}{\sqrt{1 + b_y \cdot \xi}}$$
(3.17)

with $d = 1, 1, 0.82, 0.66, 0.55, 0.55$ and $a_y = 0.22, 0.16, 0.11, 0.08, 0.06, 0.04$ for stability classes A, B, C, D, E and F respectively; $b_y = 0.0001$, α is the wind-speed exponent, and Γ is the Gamma function.

4. Formulation by Wheatley for stratified, passive flow.

Wheatley (1988) derived in a more rigorous manner the concentration distribution of a passive puff in a stratified atmosphere from an approximate solution to the diffusion equation. He arrived at an ordinary differential equation for the downwind diffusion coefficient σ_x .

ALONG-WIND-DIFFUSION FORMULATIONS IN HEGADAS

As a result of the above literature review, the following two along-wind-diffusion formulations have been implemented into HEGADAS.

1. For *non-neutral stability* an adaptation of the formulation by Ermak has been implemented. In this formulation, $\sigma_x(\xi)$ is given by

$$\sigma_x(\xi) = \sqrt{\sigma_{xs}^2 (x = \max[0, \xi - x_{br}]) + \sigma_{xt}^2 (x = \max[0, \xi - x_{br}])} \quad (3.18)$$

In the above equation σ_{xs} and σ_{xt} are defined by equation (3.17) with the wind-speed exponent chosen equal to the exponent α adopted in the HEGADAS wind-speed profile (2.1).

Note that $\max[0, \xi - x_{br}]$ equals the middle $x = 0$ of the pool for a ground-level model and it equals the downwind position x_{br} for a vertical transition plane (breakpoint).

The formulation takes into account the effect of increased shear with increased stability. However, it has a number of deficiencies. The formulation is partially based on Chatwin's formula (3.16), which strictly speaking is valid only for neutral stability and passive gas dispersion.

Moreover, in the elimination of the time the (stability-class dependent) ambient wind speed and *not* the cloud speed is adopted, and downwind diffusion is *not* ignored in regions with high Richardson numbers.

It is noted that diffusion could be ignored in regions with high Richardson number by calculating for each observer the downwind position x_{cr}^{obs} at which the Richardson number reduces to a given critical Richardson number Ri_*^{cr} (x_{cr}^{obs} corresponds to middle of pool, if $Ri_* < Ri_*^{cr}$ always) and replacing in equation (3.18) the argument $\max[0, \xi - x_{br}]$ by $\max[\xi - x_{cr}^{obs}, \xi - x_{br}]$.

However, in this manner, the σ_x -formula is no longer a direct function of x and the formulation loses its simple nature.

For these reasons the formulation may be inaccurate, particularly if high cloud concentrations occur during the dispersion processes.

2. For *neutral stability*, a heavy gas adaptation of the formulation by Chatwin for passive, neutrally stratified flow has been implemented. In this formulation σ_x is not directly related to the downwind distance ξ , but is evaluated as a function of the actual travel time t_{obs} of the cloud.

In this formulation downwind diffusion is neglected in the region where the observed bulk Richardson number Ri_*^{obs} is larger than a user-specified value Ri_*^{cr} (default value $Ri_*^{cr} = 10$), say upwind of the point x_{cr}^{obs} . As in equation (3.18), downwind diffusion is also neglected upwind of the breakpoint $x = x_{br}$.

Thus x_{cr}^{obs} is reset to x_{br} if $x_{cr}^{obs} < x_{br}$ (with x_{br} taken to be at the middle of the observed pool in the absence of a breakpoint).

The actual concentration as a function of time t and downwind distance x is determined from equation (3.13). Here the downwind dispersion coefficient σ_x is set from equation (3.16) with the time t_{obs} taken to be the travel time of the observer from x_{cr}^{obs} to ξ , i.e. $t_{obs} = t - t_{cr}^{obs}$.

In the elimination of the time the actual true speed of the puffs (observers; cloud speed) as used in HEGADAS-T is adopted, and downwind diffusion is ignored in regions with Richardson number Ri_* larger than a user-specified value Ri_*^{cr} . Therefore, in the case of neutral conditions, the adapted Chatwin formulation is more compatible with the observer concept adopted in HEGADAS-T and gives more realistic predictions than Ermak's formulation.

In the high-density region $Ri > Ri_{cr}$, downwind diffusion induced by wind shear is assumed not to take place. However, in this region considerable gravitational downwind spreading occurs which is taken into account in HEGADAS-T by the cloud-shape correction.

It is still questionable what the ideal value is to be selected for Ri_*^{cr} . The default value $Ri_*^{cr} = 10$ presently used seems to be reasonable, but may induce insufficient downwind diffusion. A higher value for Ri_*^{cr} might be more appropriate. An appropriate value for Ri_*^{cr} could be found by fitting with experimental data.

EXAMPLE

Figure 9 depicts the application of the above along-wind diffusion formulations in HEGADAS-T simulations of the Goldfish 1 experiment (constant release rate of HF for $0 < t < 125$ seconds).

This figure also includes HEGADAS-S predictions for a corresponding steady pool and HEGADAS-S predictions with a finite-duration error-function correction. Note that the amount of downwind diffusion is lower for the adapted Chatwin's formulation lower than for the adapted Ermak's formulation.

The upper envelope of the Ermak's formulation resembles the peak-concentration prediction by the error-function formulation since identical σ_x formulas are adopted in both approaches; see Section 8.6.1 in the HGSYSTEM version 1.0 Program User's Manual (Witlox, McFarlane, Rees and Puttock, 1990) for further details.

7.A.4. Interfacing with pool-evaporation and near-source jet/plume models

The user needs to supply input parameters to the heavy-gas-dispersion program HEGADAS. Among these parameters, those input data describing the near-source conditions are often not known by the user a priori.

These input data can be obtained by using one of the other models included in the HGSYSTEM software package. The models in HGSYSTEM enable the user to model a wide range of release scenarios, i.e. pressurised or unpressurised release, release of HF gas or a non-reactive ideal gas (HGSYSTEM version 1.0) or aerosol mixture (HGSYSTEM 3.0), steady-state or time-dependent (e.g. finite-duration) release rate of gas.

In the HGSYSTEM software package the program HEGADAS can be interfaced with the pool-evaporation program EVAP (HGSYSTEM 1.0) or LPOOL (HGSYSTEM 3.0) and the near-source jet/plume programs PLUME (HGSYSTEM 1.0) or AEROPLUME (HGSYSTEM 3.0) and HFPLUME.

The interfacing of HGSYSTEM modules is also discussed in Witlox and McFarlane (1994).

7.A.4.1. Interface with pool evaporation models

Liquid spillage may lead to the formation of a liquid pool. The geometry of the resulting liquid pool and the rate of evaporation can be calculated in HGSYSTEM 1.0 by the EVAP model for both steady and transient releases. EVAP calculates the (time-dependent) pool dimensions and pool evaporation rate as HEGADAS input. Chapter 4 in the HGSYSTEM version 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) includes full details on EVAP and its interface with HEGADAS.

In HGSYSTEM 3.0, EVAP has been replaced by the fully transient pool model LPOOL. Input for HEGADAS-T is generated by LPOOL. See the HGSYSTEM version 3.0 User's Manual and Chapter 4 for details on LPOOL. For releases that can be approximated as steady-state releases, the user can easily set the corresponding evaporation rate (GASFLOW or FLUX in the GASDATA input block for HEGADAS-S) in the HEGADAS-S input file. See HGSYSTEM 3.0 User's Manual for details on HEGADAS input parameters.

7.A.4.2. Interface with near-source models

For a pressurised release the heavy-gas-dispersion near the source is often momentum-dominated and HEGADAS cannot be applied in this region. Data at a near-source transition point can be derived from calculations by the near-source jet/plume models HFPLUME (for

hydrogen fluoride releases) or PLUME (for non-reactive 'ideal' gas; HGSYSTEM 1.0) or AEROPLUME (two-phase releases; HGSYSTEM 3.0). See Chapter 5 for full details on the HGSYSTEM plume models.

TRANSITION CRITERION

The plume models (AEROPLUME, HFPLUME and PLUME) simulate cloud behaviour in a near-source region. The transition from the plume models to HEGADAS is chosen at the point where the cloud conditions become more appropriate to the physical assumptions in HEGADAS. The following criteria should be satisfied simultaneously:

- The plume jet speed u^{pl} is sufficiently close to the ambient wind speed u_a at the centroid height. The ambient wind speed is adopted in the HEGADAS program to approximate the velocity.
- The total plume entrainment is sufficiently close to the heavy-gas entrainment $Entr_{gas}^{heavy}$, which is taken to be the entrainment in HEGADAS.

These criteria are included in the plume models by adding the following conditions

$$\left| u^{pl} / u_a - 1 \right| < RULST \quad \text{and} \quad 1 - Entr_{gas}^{heavy} / Entr_{total} < RELST \quad (4.1)$$

In addition to these criteria, residual buoyancy should not 'disturb' momentary advection. See Section 6.2 in Witlox, McFarlane, Rees and Puttock (1990) for a complete description of the transition criteria. See the AEROPLUME <casename>.APZ file for information on all transition criteria for the specific AEROPLUME run. This file is normally deleted but by changing the AEROPLUME.BAT file it can be saved for inspection (see section 3.5 in the HGSYSTEM 3.0 User's Manual).

The successive regions of the jet/plume flow in the plume models are the 'airborne' region (elevated jet-flow/dispersion; circular plume cross-section), the 'touchdown' region (transitional region; cut-off circle cross-section) and 'slumped' region (ground-level dispersion; semi-elliptic plume cross-section).

The transition from the plume models to the ground-level dispersion program HEGADAS can only be made following touchdown.

PLUME MODEL VARIABLES

The plume models all assume a 'top-hat' model which assumes uniform, averaged data within the jet/plume. These data are a function of the downwind distance only. The basic unknowns in the plume models are the concentration of the pollutant (plume concentration), c^{pl} , the total mixture density (plume density), ρ^{pl} , the plume speed, u^{pl} and the plume enthalpy, h^{pl} . These four unknowns are determined from four conservation equations (excess of ambient quantities), i.e. conservation of gas-mass flow, total-mass flow, extra momentum and extra energy.

At the transition point the axis inclination of the plume will be nearly horizontal. Thus the area A^{pl} of the semi-elliptic cross-section of the plume is related to the plume diameter D^{pl} and the plume centroid z_c^{pl} by

$$A^{pl} = 3 \cdot \pi^2 \cdot z_c^{pl} \cdot D^{pl} / 16 \quad (4.2)$$

See also section 5.B.6.

MATCHING OF PLUME MODEL VARIABLES WITH HEGADAS VARIABLES

The HEGADAS equations for the variables c_A , S_z , S_y , b , H_e , y_{w3} have been described in Section 2.3. These variables are set at the transition point from the plume model variables by means of appropriate matching criteria. These criteria transfer cloud characteristics and are described below.

The plume model formulation does *not* take into account heat transfer and water-vapour transfer from the ground. Thus it is consistent with the HEGADAS formulation to take $H_e = y_{w3} = 0$ at the transition point.

The plume models assume a uniform, averaged concentration within the jet. Thus it is consistent with the HEGADAS formulation to take $S_y = 0$, corresponding to a uniform concentration for $|y| < b$ and a zero concentration for $|y| > b$.

Thus the concentration c and the wind speed u adopted in HEGADAS are given at the breakpoint by (see equations (2.1) and (2.2))

$$c(x, y, z) = c_A \exp \left[- \left(\frac{z}{S_z(x)} \right)^\beta \right], \quad |y| < b, \quad u = u_0 \left(\frac{z}{z_0} \right)^\alpha \quad (4.3)$$

with $\beta = 1 + \alpha$.

It remains to determine the variables c_A , S_z and b in equation (4.3). One might determine these variables by imposing the conservation equations adopted in the plume models.

Conservation of extra momentum is not applicable, because HEGADAS assumes the velocity to be the ambient wind speed (zero extra momentum).

Conservation of extra energy seems not to be appropriate because by setting $H_e = 0$ in HEGADAS we actually have ignored heat effects at the transition point.

Instead the following three conditions are imposed to determine the variables c_A , S_z and b :

- o Conservation of pollutant mass flow.

This means that the total flow of pollutant (kg/s), E , flowing through the transition plane $x = x_{br}$ is preserved. E is given by the following integral as a 'first' moment M_1 in concentration:

$$E = M_1 = \int_0^{\infty} \int_{-\infty}^{\infty} u c \, dy \, dz \quad (4.4)$$

- o Conservation of total plume mass.

This means that the flow of total plume mass (kg/s) is conserved. The total mass flow M_{tot} is given by

$$M_{tot} = \int_0^{\infty} \int_{-\infty}^{\infty} u \rho \, dy \, dz \quad (4.5a)$$

where ρ is the plume density.

However, an expression involving the concentration c is needed as this is one of the matching variables. For small concentrations, the total density ρ can be written as a function $\rho(c)$ of $c(z)$. Using a Maclaurin expansion around $c = 0$ for small c ,

$$\rho(c) = \rho(0) + c\rho'(0) + \frac{1}{2}c^2\rho''(0) + H.O. \quad (4.5b)$$

where H.O. stands for higher order terms. Inserting (4.5b) into (4.5a) it can be concluded that for $c \rightarrow 0$, conservation of total mass is implied by conservation of pollutant mass equation (4.4) (the term linear in c) and conservation of the 'second' moment M_2 of concentration (the quadratic term in c):

$$M_2 = \int_0^{\infty} \int_{-\infty}^{\infty} u c^2 dy dz \quad (4.5c)$$

o Plume centroid height.

The centroid height z_c is given by

$$z_c = \frac{1}{M_1} \cdot \int_0^{\infty} \int_{-\infty}^{\infty} u c z dy dz \quad (4.6)$$

Both the HEGADAS similarity profile (4.3) and the plume model top-hat profile for c and u are now inserted into the above conditions (4.4), (4.5) and (4.6). Subsequent matching leads to the following three conditions:

$$M_1 = A^{pl} \cdot c^{pl} \cdot u^{pl} = \frac{2}{\beta} \cdot \Gamma\left(\frac{1+\alpha}{\beta}\right) \cdot \frac{S_z^{1+\alpha}}{z_0^\alpha} b \cdot c_A \cdot u_0 \quad (4.7)$$

$$M_2 = A^{pl} \cdot (c^{pl})^2 \cdot u^{pl} = 2^{-\frac{(1+\alpha)}{\beta}} \cdot \frac{2}{\beta} \cdot \Gamma((1+\alpha)/\beta) \cdot \frac{S_z^{1+\alpha}}{z_0^\alpha} b \cdot (c_A)^2 \cdot u_0 \quad (4.8)$$

$$z_c = z_c^{pl} = S_z \cdot \Gamma((2+\alpha)/\beta) / \Gamma((1+\alpha)/\beta) \quad (4.9)$$

In HEGADAS the exponent β in the vertical concentration profile is related to the wind-speed exponent α by $\beta = 1+\alpha$ (see equation 2.2). From HEGADAS simulations of experiments it is known that HEGADAS accurately predicts ground-level concentrations, but often badly predicts vertical variations of the concentration. Thus in the matching process it is not appropriate to adopt $\beta = 1+\alpha$ to obtain from the HFPLUME (uniform) data accurate estimates of the parameters c_A and b that determine the ground-level concentration. Instead, in particular in the far-field, a Gaussian concentration profile defined by $\beta = 2$ will be more appropriate.

Moreover the wind speed $u(z)$ is approximated by the (uniform) centroid plume speed.

Thus $u(z) = u^{pl} = u_0 \cdot (z/z_0)^\alpha$, $\alpha = 0$, $\beta = 2$ are inserted in the above matching conditions (4.7), (4.8) and (4.9). By eliminating z_c^{pl} and using equation (4.2), the following conditions are then derived:

$$c_A = \sqrt{2} \cdot c^{pl} \quad (4.10)$$

$$b = \frac{3 \cdot \pi}{16 \cdot \sqrt{2}} \cdot D^{pl} \quad (4.11)$$

Finally the HEGADAS variable S_z is set from the gas-mass conservation equation (2.8) with the value of β taken to be consistent with the HEGADAS assumption $\beta = 1 + \alpha$.

SENSITIVITY TO TRANSITION CRITERIA

Figure 10 illustrates the effect of the transition criteria (4.1) on the HFPLUME/HEGADAS predictions.

In agreement with equation (4.10) the HFPLUME (sectional-mean) concentration curves are almost parallel at the transition point to the HEGADAS (centre-line, ground-level) concentration curves.

The cloud half-width in Figure 10b equals $B_{\text{eff}} = 3 \cdot \pi \cdot D^{pl} / (16 \cdot \sqrt{2})$ in the HFPLUME region [compare equation (4.11)] and $B_{\text{eff}} = b + \frac{1}{2} \cdot \sqrt{\pi} \cdot S_y$ in the HEGADAS region [see equation (2.4)].

The concentration predictions are almost unaffected by the precise position of the transition point if $RULST < 0.1$ and $RELST < 0.3$. The values $RULST = 0.1$ and $RELST = 0.3$ are recommended and are default values in HGSYSTEM (versions 1.0 and 3.0).

7.A.5.3. Interface with near-source models (finite-duration release)

For the same reasons as for HEGADAS-S, the time-dependent model HEGADAS-T may not be applied to pressurised releases in the high-momentum near-source region. Thus HEGADAS-T should be only applied downwind of an appropriately chosen transition point or breakpoint $x = x_{br}$.

For *finite-duration releases* the program HEGADAS-T can automatically be interfaced with the near-source plume models. To this purpose the (steady-state) transition data are applied at the breakpoint x_{br} for a period corresponding to the release duration T_{dur} .

Thus at the breakpoint x_{br} , the dry-pollutant flow E (kg/s), the centre-line ground-level pollutant molar fraction y_{pol} (from equation (4.10) and the relevant thermodynamic model) and the cloud half-width b (m; from equation (4.11)) are applied for a period of T_{dur} (s).

Gas is being released at the release point $x = 0$ during the period $0 < \text{time } t < T_{dur}$. In applying the above transition data at $x = x_{br}$ one must take into account the travel time T_{br} of the plume between the release point $x = 0$ and the transition point $x = x_{br}$. Thus the transition data are

applied for $T_{br} < \text{time } t < T_{br} + T_{dur}$. The travel time T_{br} can be expressed in terms of the plume speed $u = u(x)$ by the following formula,

$$T_{br} = \int_0^{x_{br}} \frac{1}{u_x(x)} dx \quad (4.12)$$

where $u_x(x)$ is the horizontal component of the plume speed u^{pl} .

7.A.5. Validation

The physics or fundamentals of the HEGADAS model described in the previous sections were developed using experimental laboratory data. Parameters which quantify a particular physical process have been determined, where possible, from laboratory experiments which study that process in isolation. This has been carried out as follows.

- The empirical formula (2.10) for the entrainment velocity is based on data for a large number of wind tunnel experiments (see Section 7.A.2.3).
- The initial crosswind spreading law (2.12a) is based on experiments by Van Ulden (1984), and the subsequent collapse of gravity spreading given by equations (2.12b) and (2.12c) is based on experiments by Linden and Simpson (1988). The crosswind diffusion given by equations (2.13) and (2.13*) is based on empirical formulae for the non-dense crosswind dispersion coefficient σ_y introduced by Briggs (1973).
- The empirical formula (C.2 in Appendix 7.A.C) for the heat flux Q_H in the heat equation (2.14) is based on expressions for the forced and natural convection heat flux proposed by Holman (1981) and McAdams (1954).
The water-vapour equation (2.15) is based on a theoretical approach by Rosner (1967). equations (2.14) and (2.15) have been validated by Colenbrander and Puttock (1984) by means of a series of three experiments involving cold nitrogen flowing across a water surface. See Section 5 of Appendix 3 of the HGSYSTEM 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) for further historical details.
- The hydrogen fluoride thermodynamics formulation described in Chapter 2.B. is based on experimental data by Schotte (1987,1988); see Figure 4.

The HEGADAS model was then validated against independent wind-tunnel and field data to ensure that it correctly describes the effect of these various physical processes in combination.

Thus an independence is maintained between the model formulation and the data which is used to verify the model (i.e. HEGADAS is not tuned to any particular field data set).

By using this approach, greater confidence can be given to the predictions from the HEGADAS model. The HEGADAS model was validated against the following wind-tunnel and field data.

1. Puttock, Colenbrander and Blackmore (1984) modelled continuous releases of liquid propane and LNG over water in the Maplin Sands field experiments (HEGADAS-2 version). Figure 11 illustrates the improved predictions for Maplin Spill 54 by the HEGADAS-5 version as available in HGSYSTEM 1.0.
2. Roberts (see Chapter 8 in the HGSYSTEM 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) for historical details) modelled wind tunnel data by Petersen and Ratcliff (1989) for steady, isothermal dispersion (HEGADAS-5; Figure 2). These experiments involved a wide range of surface roughnesses and gas/air density ratios.
3. Colenbrander and Puttock (1984) modelled transient releases of liquid propane and LNG over water in the Maplin Sands field experiments while including both heat and water-vapour transfer from the substrate (HEGADAS-4 version; Figure 12).
4. Puttock (1987) modelled instantaneous releases of Freon in Thorney Island experiments (Figure 13). He modelled the gravity-slumping in the near-field by the box model HEGABOX (see Chapter 8) and the dispersion further downwind was modelled by HEGADAS-T (HEGADAS-4 version).
5. Witlox (see Chapter 9 in the HGSYSTEM Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) for full historical details) modelled steady and finite-duration pressurised releases of HF for the Goldfish experiments (Blewitt, 1988). He modelled the near-field momentum-dominated dispersion using the HGSYSTEM model HFPLUME and the dispersion further downwind by HEGADAS-5. Figures 14 and 15 illustrate the steady-state dispersion predictions for the Goldfish 3 experiment. Figures 8 and 9 illustrate the finite-duration dispersion predictions for the Goldfish 1 experiment.

The intended application of HEGADAS is to simulate postulated accidental releases of a hazardous pollutant in an industrial setting. However, there is no one set of experimental data

against which all aspects of the model can be tested in its entirety. In verifying the models sensitivity analyses are the only method of testing the interaction of all components of the models and the validity of the several model assumptions. From these analyses it can be ensured that the results are physically reasonable. For the pressurised release of HF a detailed sensitivity analysis was carried out by Witlox. In this sensitivity analysis the near-field momentum-dominated dispersion was modelled by the HGSYSTEM model HFPLUME and the dispersion further downwind by HEGADAS.

The sensitivity to both input variables (meteorological data, source data, etc.) and model assumptions (interface criteria, crosswind-spreading and diffusion formulations, ..) were investigated. Two base cases were considered, one case with conditions similar to the Goldfish 2 experiment (high temperature, low surface roughness and humidity) and one with more typical rural conditions. See Chapter 10 in the HGSYSTEM 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) for full historical details.

7.A.6. Summary and conclusions

This report includes a complete technical description of the heavy-gas-dispersion model HEGADAS-5 as it was provided in HGSYSTEM version 1.0.

A number of enhancements and extensions to similarity models for heavy gas dispersion problems have been described, which have been incorporated into the HEGADAS-5 version of HEGADAS.

HEGADAS is based on an empirical similarity profile for the concentration, which is expressed in terms of the centre-line ground-level concentration and vertical/cross-wind dispersion parameters. The latter quantities are determined from a number of basic equations describing gas-mass conversation, air entrainment, cross-wind gravity spreading and cross-wind diffusion. The model includes the following new features:

1. A cross-wind gravity-spreading formulation, which accounts for the phenomenon of collapse of gravitational spreading (Section 7.A.2.3)
2. A generalised cross-wind diffusion law for improved prediction of cross-wind diffusion far downwind (e.g. possibility of Briggs formula for cross-wind dispersion coefficient σ_y ; Section 7.A.2.3 and Appendix 7.A.B).
3. A thermodynamical description for HF, which takes into account the effects of polymerisation and the exothermic reaction of HF with the water-vapour in the moist air (Chapter 2.B).

4. A new algorithm for evaluation of the concentration data for transient releases (Section 7.A.3.2).
5. An improved formulation describing the spreading and evaporation of the pool (gas-blanket formulation) for transient releases (Section 7.A.3.3).
6. A new formulation with time-dependent dispersion calculations being started from a transition plane with a near-field jet model (Section 7.A.3.4). Thus the heavy-gas-dispersion model can be interfaced with near-source jet/plume models for time-dependent pressurised releases.
7. An improved formulation describing the inclusion of along-wind-diffusion effects for transient releases (Section 7.A.3.5).
8. A fully automated interface of the steady or transient heavy-gas dispersion model with pool-evaporation models (for unpressurised releases; Section 7.A.4.1) or with near-source jet/plume models (at a given transition point; for pressurised releases; Sections 7.A.4.2 and 7.A.4.3).

These model enhancements have been validated by simulating the HTAG wind-tunnel experiments (steady unpressurised release of ideal gases) and the Goldfish experiments (steady and finite-duration pressurised release of HF).

The program has also been evaluated by a sensitivity analysis (steady pressurised release of HF).

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ACKNOWLEDGEMENT

Some of the work reported here has been carried out as part of the Industry Co-operative HF Mitigation/Assessment Program. This program has been sponsored and funded by Allied-Signal, Amoco, Ashland, Chevron, Conoco/DuPont, Dow, Elf Aquitaine, Exxon, Kerr-McGee, Marathon, Mobil, Phillips, Saras, Shell International, Sohio, Sun, Tenneco, Texaco, Unocal and 3M.

7.A.8. Notation

This section contains a list of the major symbols used in the report. For each symbol the meaning and unit of the symbol is given, and the number of equation or section where it is defined. The sections and appendices are indicated without the 7.A prefix.

<u>Symbol</u>	<u>Meaning and unit</u>	<u>Reference</u>
$b(x)$	half-width of middle part of crosswind concentration profile (m); $b = 0$ after profile has become Gaussian	Eq. (2.2)
B	half-width of secondary ground-level pool (m)	Sect. 2.4
$B_{\text{eff}}(x)$	effective cloud half-width (m)	Eq. (2.4)
B_p	half-width of primary ground-level pool (m)	Sect. 2.4
$c(x,y,z)$	dry-pollutant concentration (kg/m^3)	Eq. (2.2)
$c_A(x)$	dry-pollutant centre-line ground-level concentration (kg/m^3)	Eq. (2.2)
c_p^α, C_p^α	specific heat ($\text{J}/\text{kg}/\text{K}$ and $\text{J}/\text{kmole}/\text{K}$, respectively) of species α [$\alpha = dp, a, N, wl, wv, wi$ for dry pollutant, air, N-gas, water vapour, water liquid and ice]	App. C.2

E	dry-pollutant source emission rate (kg/s)	Eq. (2.8)
$E_{\max}(B,L)$	maximum take-up rate (kg/s) of dry pollutant for ground-level source with half-width B and length L == emission rate of gas blanket with dimensions B,L	Eq. (2.16)
g	gravitational acceleration (= 9.81 m/s ²)	Eq. (2.11)
H_{cond}^w	heat of condensation of water (Joule/kmole)	App. D
H_{fus}^w	heat of fusion of water (Joule/kmole)	App. D
$H_e(x)$	heat added from the substrate to the pollutant/air mixture (J/kmole)	Sect. 2.2
$H_{\text{eff}}(x)$	effective cloud height (m)	Eq. (2.5)
L	length of secondary ground-level pool (m)	Sect. 2.4
L_p	length of primary ground-level pool (m)	Sect. 2.4
m_α	molecular weight of species α [$\alpha = dp, w, a, amb$ for dry pollutant, water, dry air and ambient air, resp.]	Sect. 2.2
$M_{\text{eff}}^{\text{mol}}(x)$	effective molar cloud flow (kmole/s of mixture flowing through vertical plane at downwind distance x)	Eq. (2.7)
P	total pressure (atm); in HEGADAS always taken to be 1	
$P_w^w(T)$	saturated vapour pressure of water (atm) at temperature T (in °C)	Eq. (A.13)
$Q_H(x)$	heat flux from substrate to cloud (J/s/m ²)	Eq. (2.14)
$Q_{wv}(x)$	water-vapour flux from substrate to cloud (kmole/s/m ²)	Eq. (2.15)
r_H	relative humidity of air (fraction; $0 < r_H < 1$)	Eq. (A.12)
R	gas constant = 0.082 atm/K/kmole = 8314.3 J/K/kmole	
$Ri_s(x)$	bulk Richardson number (-)	Eq. (2.11)
$Ri(x)$	Richardson number (-)	Eq.(2.12b)
$S_y(x)$	crosswind dispersion coefficient (m)	Eq. (2.2)
$S_z(x)$	vertical dispersion coefficient (m)	Eq. (2.2)
T_a	ambient temperature at ground level (°C)	App. A
$T_m(x)$	centre-line ground-level mixture temperature (°C)	App. A
T_{pol}	pollutant temperature (°C)	App. D
T_s	substrate temperature (°C)	App. C
u(z)	ambient wind speed (m/s)	Eq. (2.1)
$u_{\text{eff}}(x)$	effective cloud speed (m/s)	Eq. (2.6)
$u_T(x)$	modified friction velocity (m/s) to account for air entrainment caused by convected advents due to temperature differences between substrate and cloud	Eq. (C.11)
u_0	ambient velocity at reference height z0	Eq. (2.1)
u^*	ambient friction velocity (m/s)	Eq. (A.1)
V_0	volume of ideal gas at 0 °C and 1 atm. (= 22.4 m ³ /kmole)	Eq. (2.9)
$V_m(x)$	centre-line ground-level mixture volume (m ³ /kmole)	Eq. (2.3)

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x	downwind distance from middle of pool (m)	Sect. 2.1
x_{br}	x co-ordinate of transition plane (breakpoint) between HEGADAS and near-source dispersion model	Sect. 5.2
y	crosswind distance from centre-line of cloud (m)	Sect. 2.1
$y_{pol}(x)$	centre-line ground-level pollutant molar fraction (-)	Eq. 2.3
$y_{w3}(x)$	water-vapour added from the substrate (kmole/kmole of mixture)	Sect. 2.2
z	vertical height above substrate (m)	Sect. 2.1
z_0	reference height for ambient velocity u_0 (m)	Eq. (2.1)
z^R	surface roughness (m)	Eq. (A.1)
α	exponent in power-law fit of ambient wind-speed (-)	Eq. (2.1)
β	exponent in concentration similarity profile (-)	Eq. (2.2)
η_w	mole fraction of water in pollutant (-)	Eq. (2.8)
κ	Von Kármán constant = 0.41 (-)	Eq. (A.1)
λ	Monin-Obukhov length (m)	Eq. (A.1)
$\rho_{amb}(z)$	ground-level density of moist ambient air (kg/m^3)	Eq. (A.10)
$\rho_m(x)$	centre-line ground-level mixture density (kg/m^3)	Sect. 2.2
$\sigma_x(x)$	downwind dispersion coefficient (m)	Eq. (3.13)
$\Phi(Ri_*)$	empirical entrainment function (-)	Eq. (2.11)

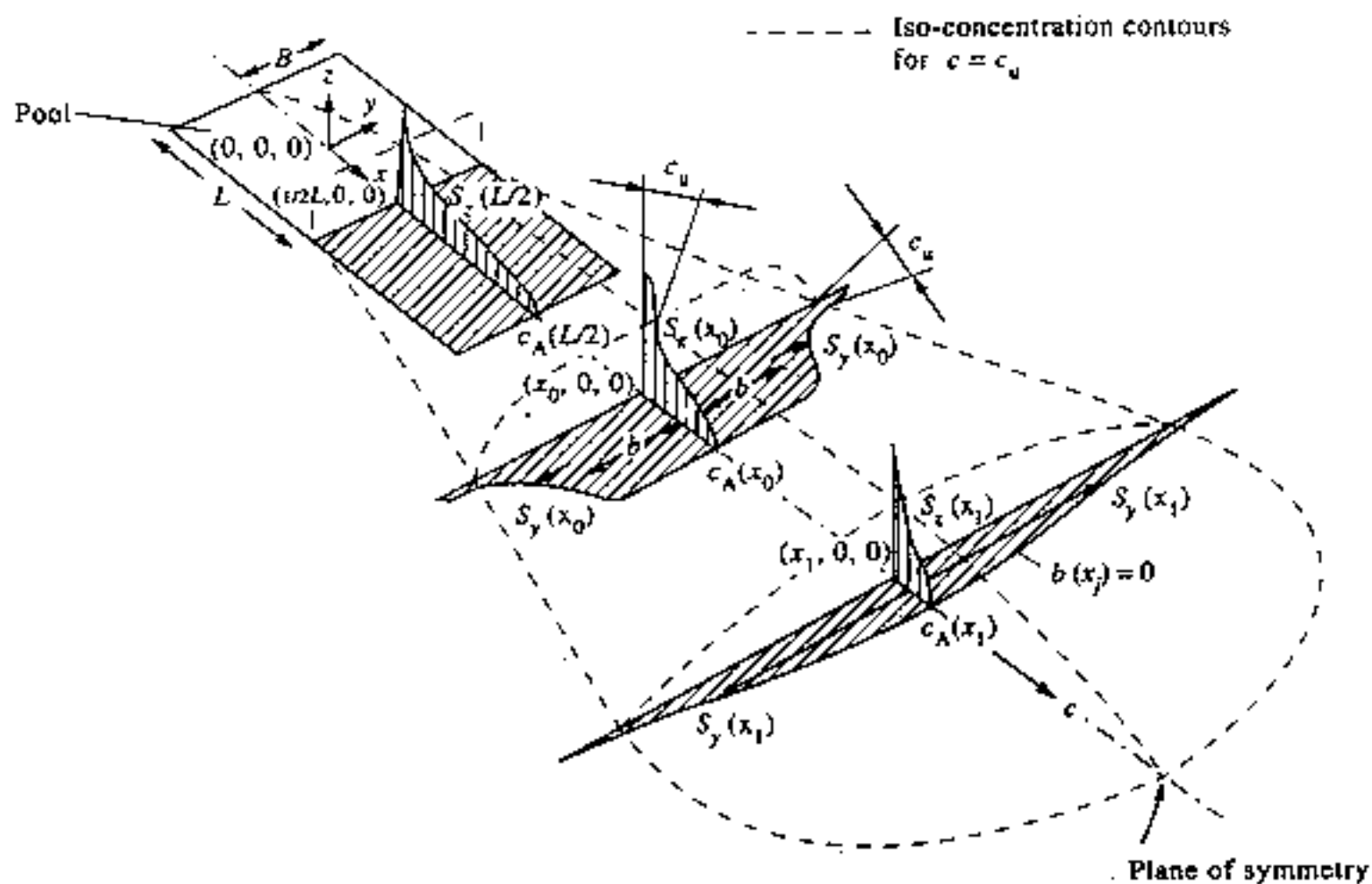


FIG. 1 - The HEGADAS similarity profile for the concentration $c(x,y,z)$; c_A is the centre-line ground-level concentration, b the crosswind half-width along which the ground-level concentration equals c_A , S_y the crosswind dispersion coefficient defining the Gaussian decay in concentration at larger crosswind distances, and S_z the vertical dispersion coefficient defining the vertical decay; B is the half-width and L is the length of the ground-level pool. The figure includes also iso-concentration contours (dashed lines) in the planes $y=0$, $z=0$, $x=1/2L$, $x=x_0$ and $x=x_1$

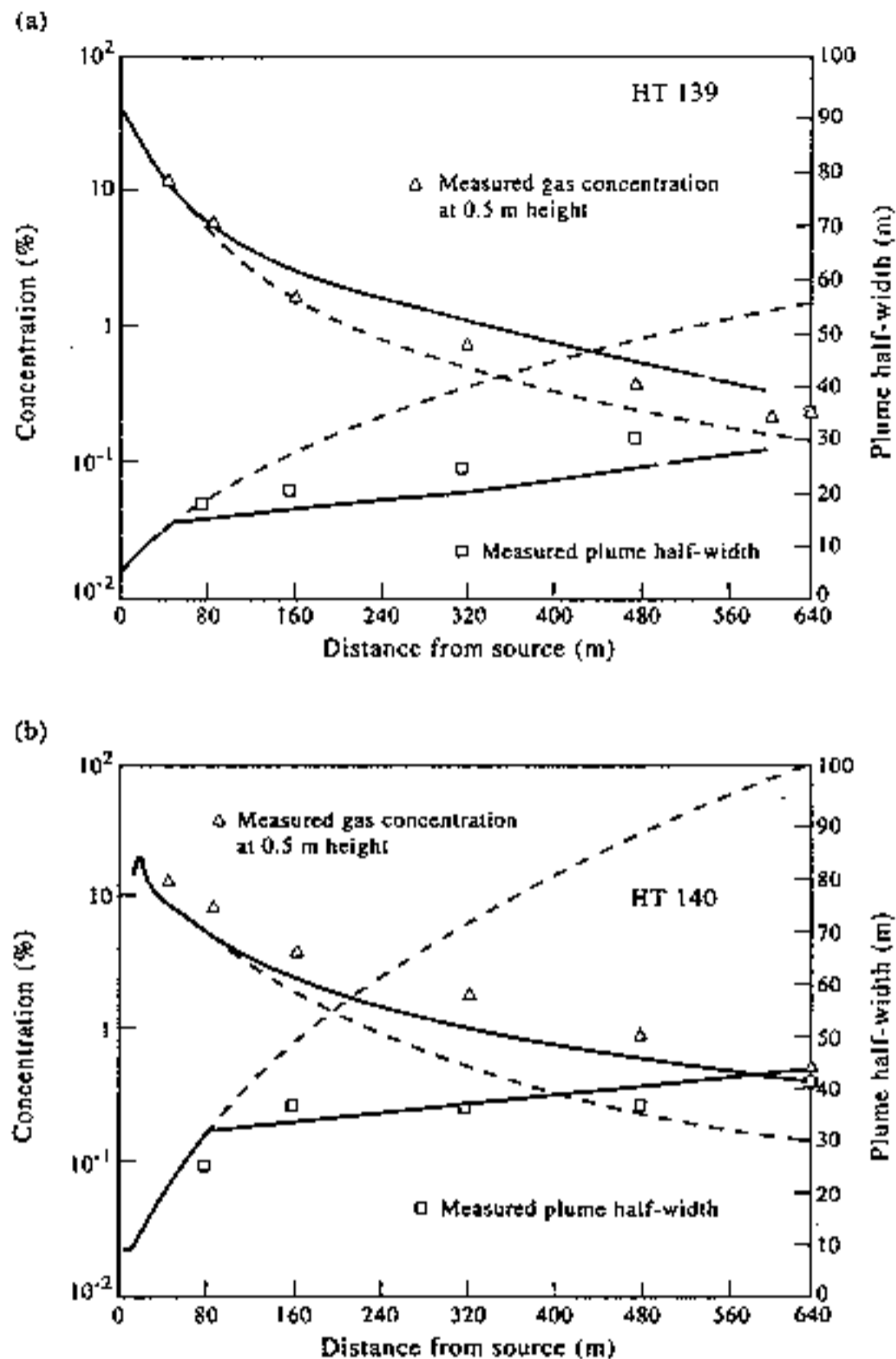


FIG. 2 - Effect of changing the gravity-spreading formulation in HEGADAS to describe the plume spread observed in the HTAG dispersion experiments (see McFarlane et al. (1990)). The dashed lines show the plume widths and centre-line concentrations predicted by the HEGADAS-4 model. The HTAG data (squares) shows a sharp reduction in the plume spread at about 80 m. The solid lines show the revised HEGADAS-5 model predictions that take this into account;

(a) surface roughness = 0.03 m, gas/air density ratio = 1.4,

(b) surface roughness = 0.03 m, gas/air density ratio = 3.9.

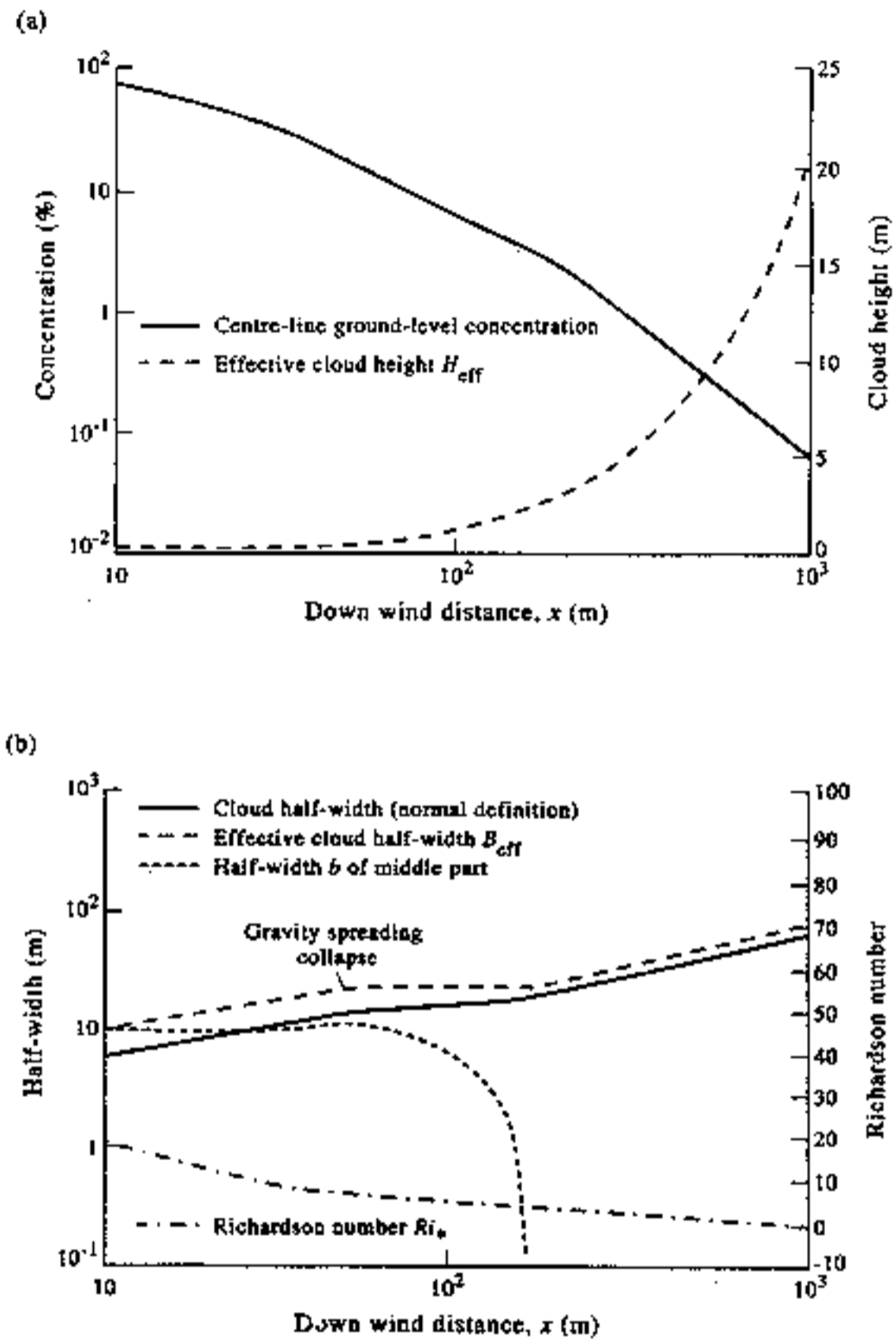


FIG. 3 - HEGADAS-S dispersion predictions from ground-level pool of propane located at $x=0$ (evaporation rate $E = 32$ kg/s):
 (a) centre-line ground-level concentration (molar fraction),
 (b) cloud half-width, effective half-width B_{eff} , and half-width b of uniform section of concentration profile

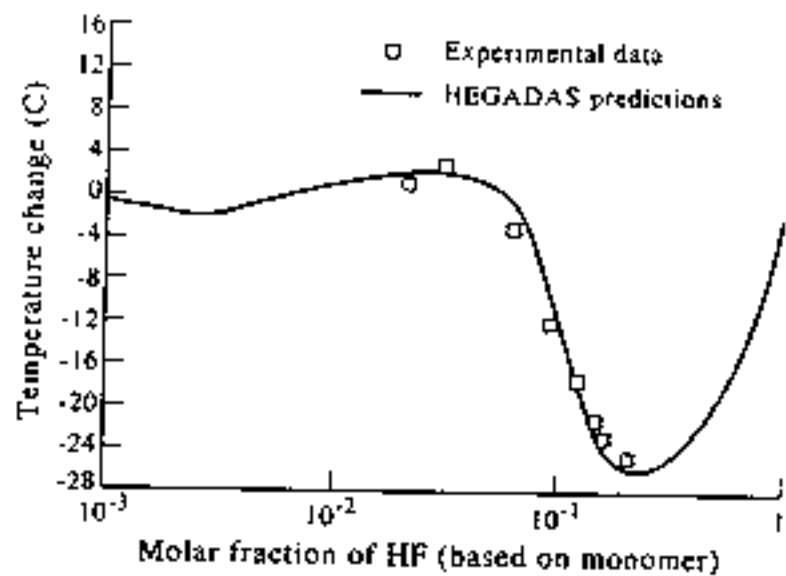


FIG. 4 - Mixing of anhydrous HF with moist air (relative humidity = 50%) at 26°C; experimental data from Schotte (1987) and HEGADAS-5 predictions of change in temperature $\Delta T = T - 26$ as a function of the molar fraction y_{pol} of HF

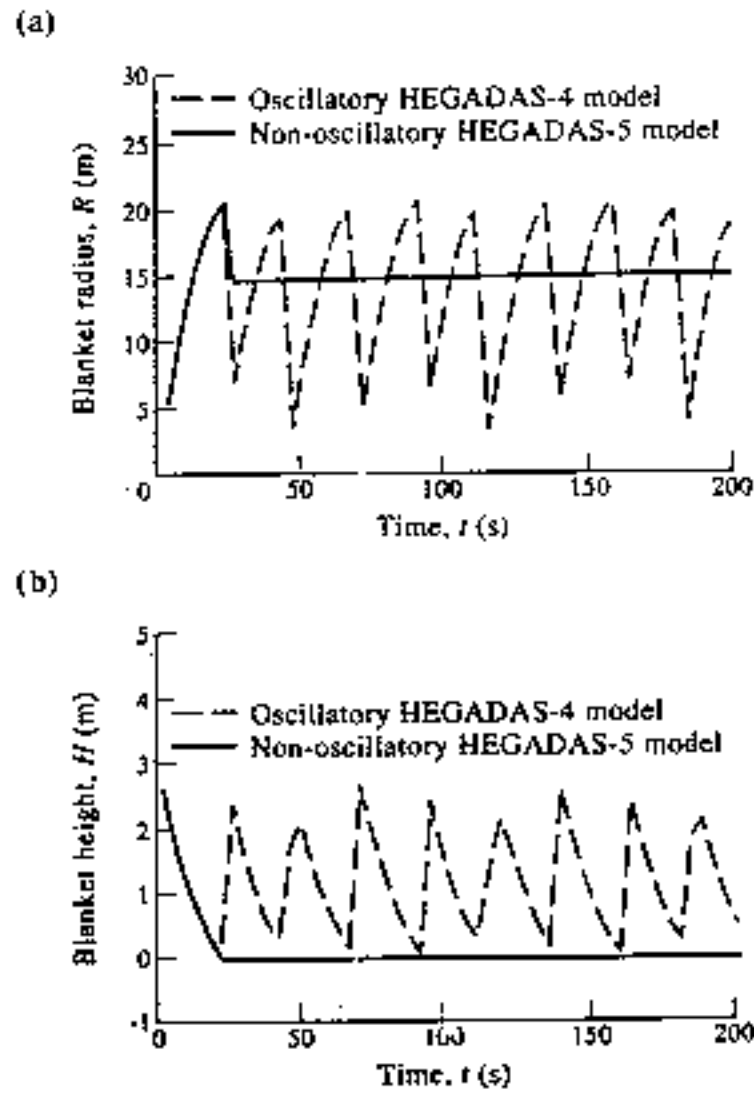


FIG. 5 - Vapour source from a boiling propane pool of radius $R_p = 3$ m, evaporation rate $E = 30$ kg/s and spill duration = 200 seconds; gas-blanket predictions by HEGADAS-4 and HEGADAS-5 models;

(a) blanket radius $R_g(t)$

(b) blanket height $H_g(t)$

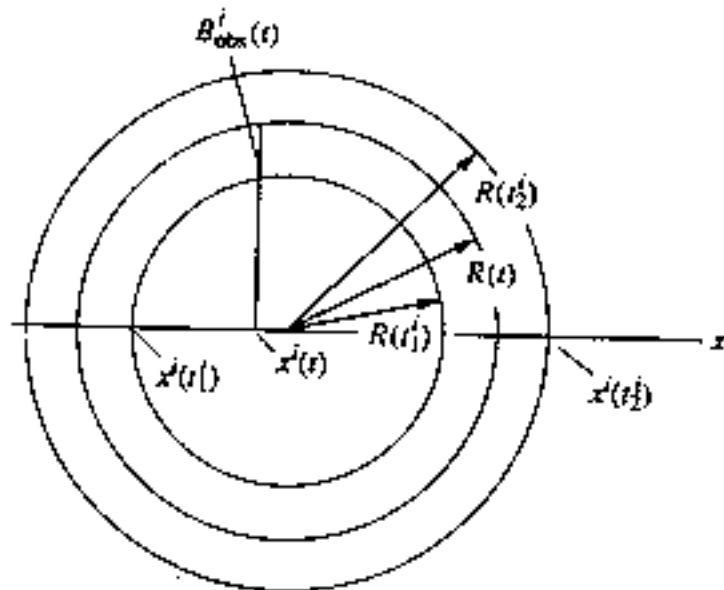


FIG. 6 - Movement of observer i over time-dependent secondary source. Observer i passes over the upwind and downwind edges of the source at times $t=t_1^j$ and $t=t_2^j$. At time t ($t_1^j < t < t_2^j$), observer i is located at $x^j(t)$, and sees a source width $B_{obs}^i(t) = [R^2(t) - x^j(t)x^j(t)]^{1/2}$, and a source flux $Q(t)$

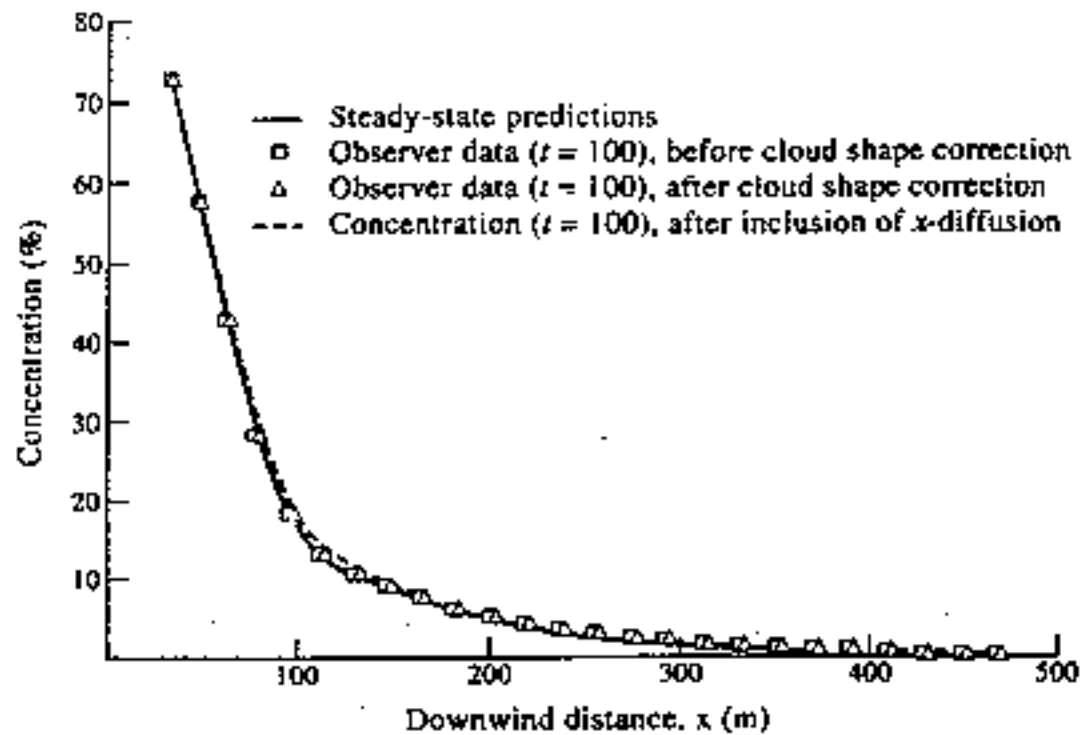


FIG. 7 - HEGADAS-T predictions of centre-line ground-level concentration (% molar fraction) at time $t = 100$ s for finite-duration steady flow of propane through the transition plane $x_{tr} = 30$ m (propane flow $E(t) = 32$ kg/s, $0 < t < 100$) and HEGADAS-S predictions for corresponding steady flow ($E = 32$ kg/s)

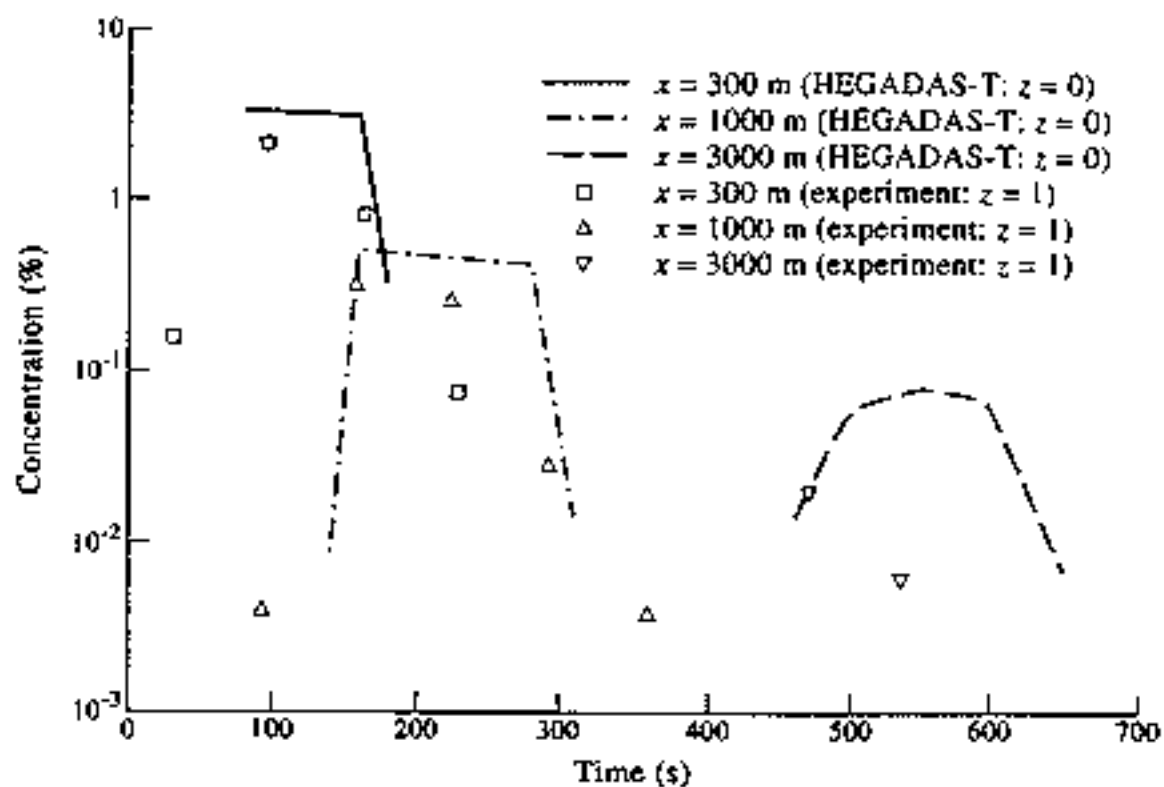


FIG. 8 - HEGADAS-T simulation of Goldfish 1 experiment (steady pressurised release of anhydrous HF for 125 seconds); HEGADAS-T simulation is started from transition plane at 188 m with transition data derived from the near-source model HFPLUME. Experimental data at 3000 m are too low, since the centre-line of the plume was not aligned with the line on which the concentration measurements were made

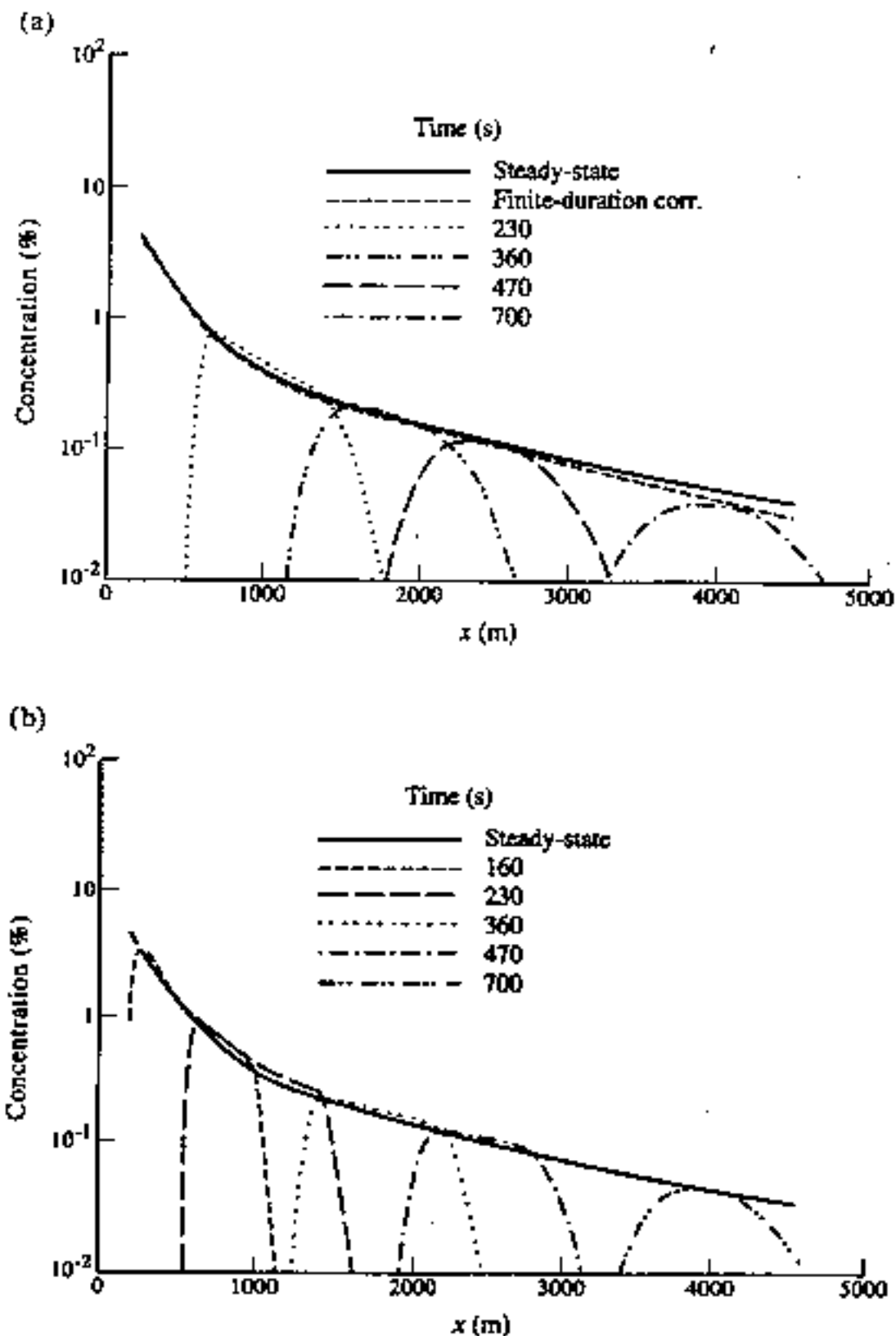


FIG. 9 - HEGADAS simulation of Goldfish I experiment (HF-release rate of $E = 27$ kg/s for 125 seconds; HFPLUME/HEGADAS transition data at 188 m). Comparison of HEGADAS-S steady-state predictions, HEGADAS-S/HSPOST steady-state predictions with finite-duration error-function correction and HEGADAS-T time-dependent predictions:
 (a) use of adapted Ermak's σ_x - formulation in HEGADAS-T
 (b) use of adapted Charwin's σ_x - formulation in HEGADAS-T

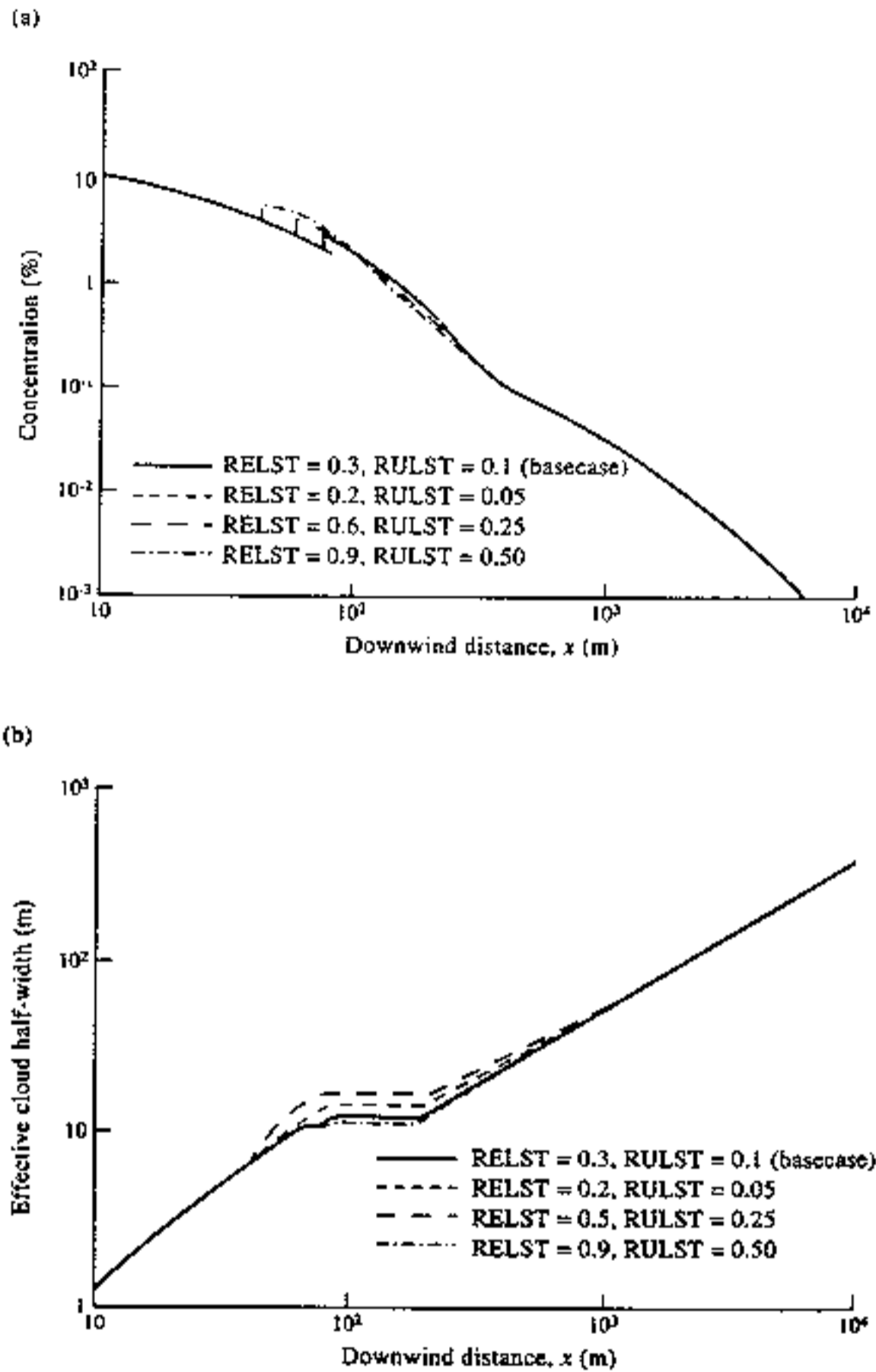


FIG. 10 - Steady pressurised release of HF under typical rural conditions; effect of variation of HFPLUME/HEGADAS-S transition criteria; transition from HFPLUME to HEGADAS-S is made if the proportion of heavy-gas entrainment in the total entrainment is larger than $(1 - \text{RELST}) \cdot 100\%$ and the difference in plume speed and ambient speed is less than $\text{RULST} \cdot 100\%$; recommended values are RELST = 0.03 and RULST = 0.1:

(a) centre-line concentration (% molar fraction: HFPLUME sectional-mean value and HEGADAS value at ground-level)

(b) effective half-width E_{eff} of cloud

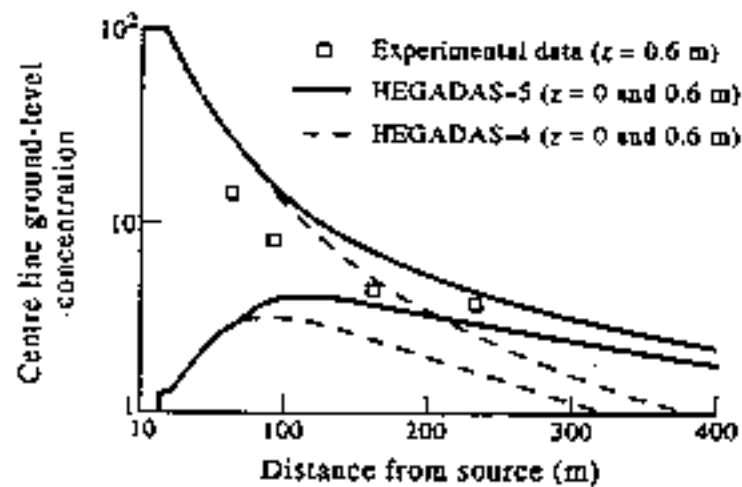


FIG. 11 - Steady dispersion of propane over water (Maplin Spill 54). HEGADAS-4 and HEGADAS-5 predictions of centre-line ground-level concentration (% molar fraction)

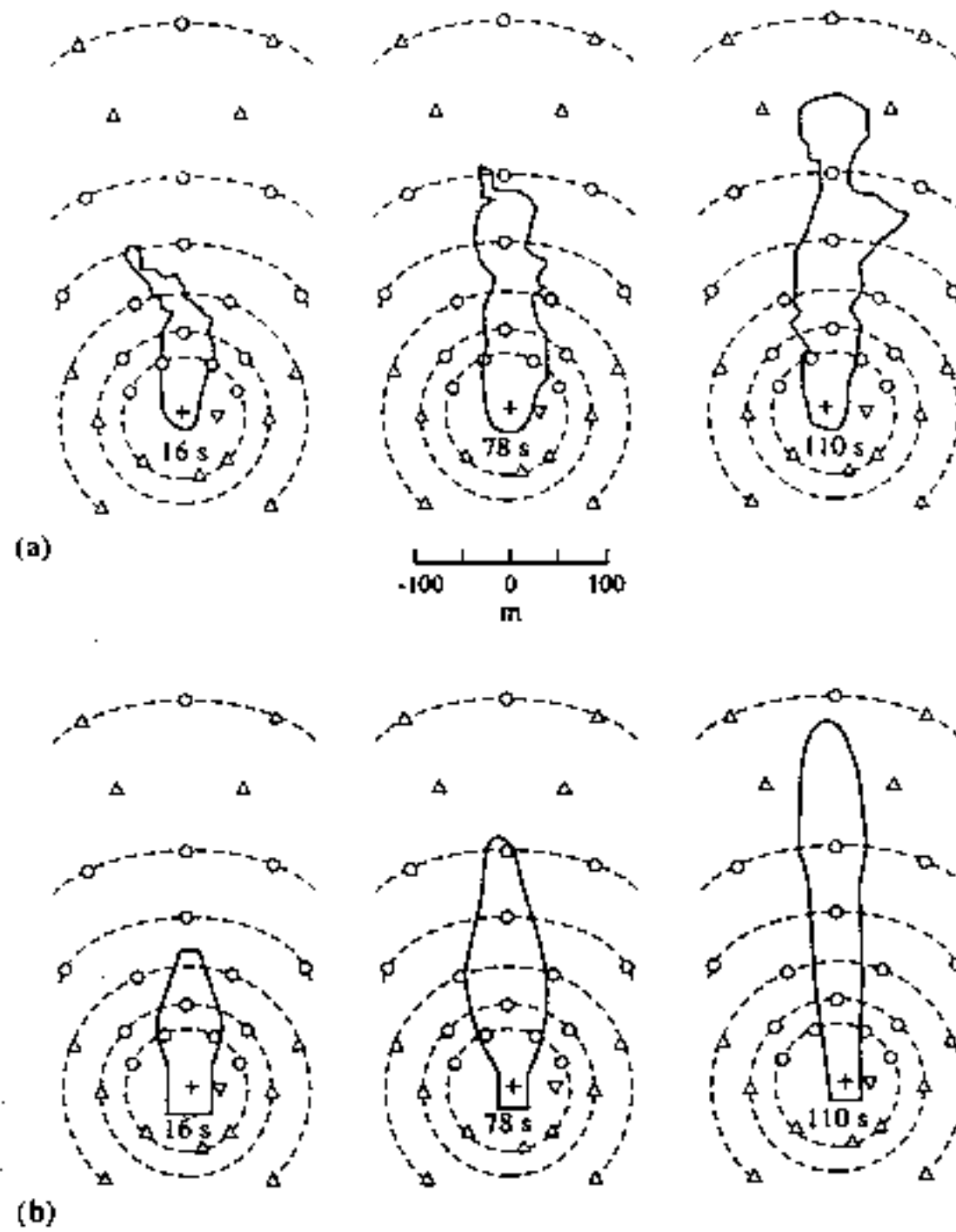


FIG. 12 - Time-dependent dispersion of LNG over water (Maplin Spill 22: release of 10 m^3): 3% concentration contours

(a) experimental data at times $t = 16, 78$ and 110 s

(b) HEGADAS-4-T predictions at times $t = 16, 78$ and 110 s

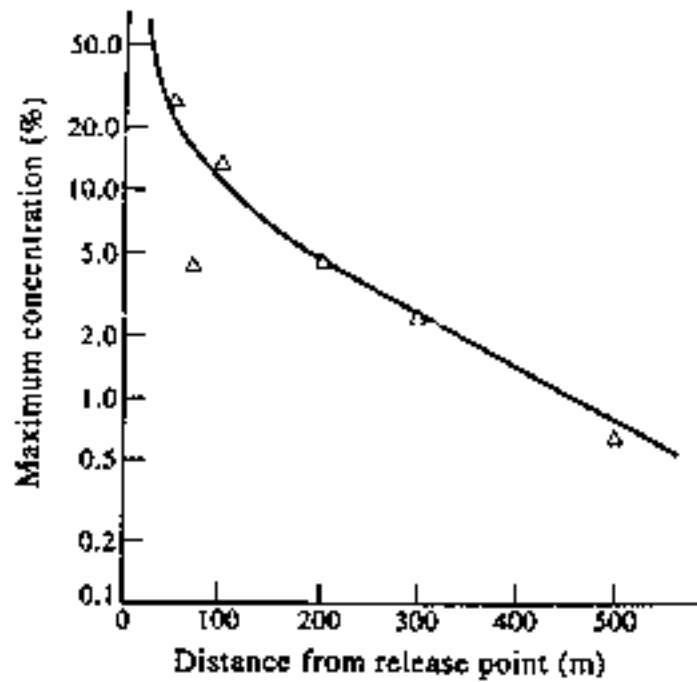


FIG. 13 - Instantaneous release of Freon (Thorney Island trial 15): observed peak concentrations at 0.4 m height versus HEGABOX/HEGADAS centre-line ground-level predictions

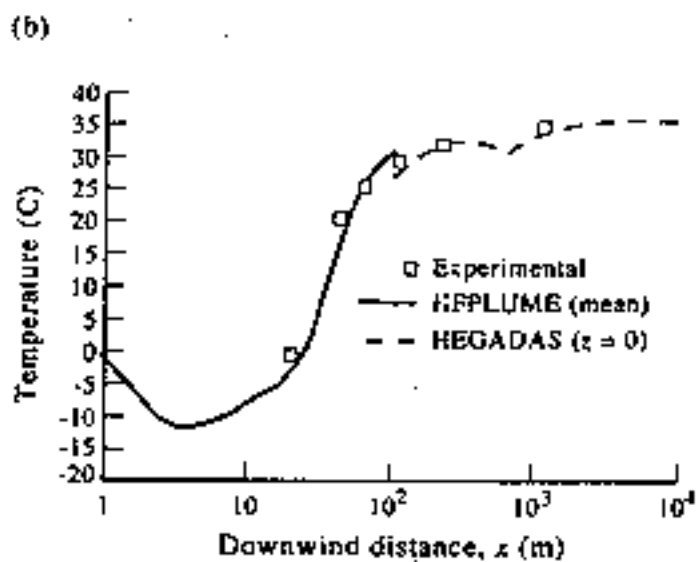
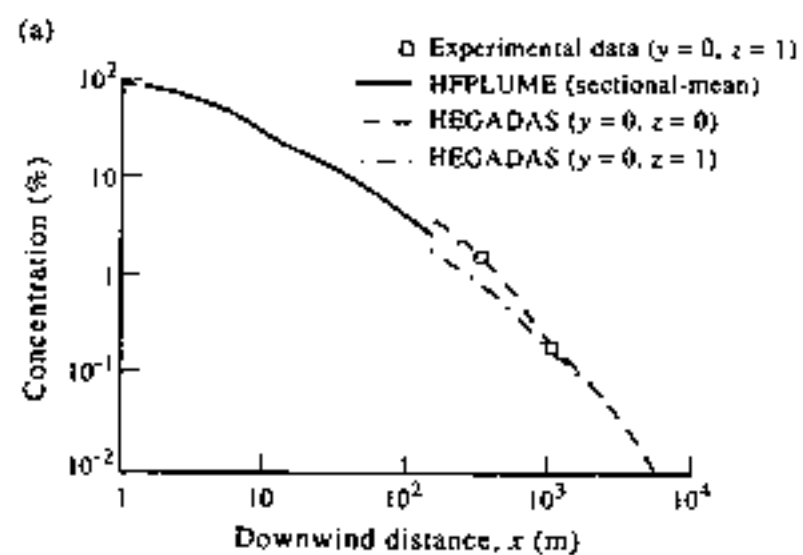


FIG. 14 - Simulation of Goldfish 3 experiment (steady pressurised release of anhydrous HF) by the near-source model HFPLUME and the heavy-gas-dispersion model HEGADAS-S;
 (a) centre-line concentration
 (b) temperature

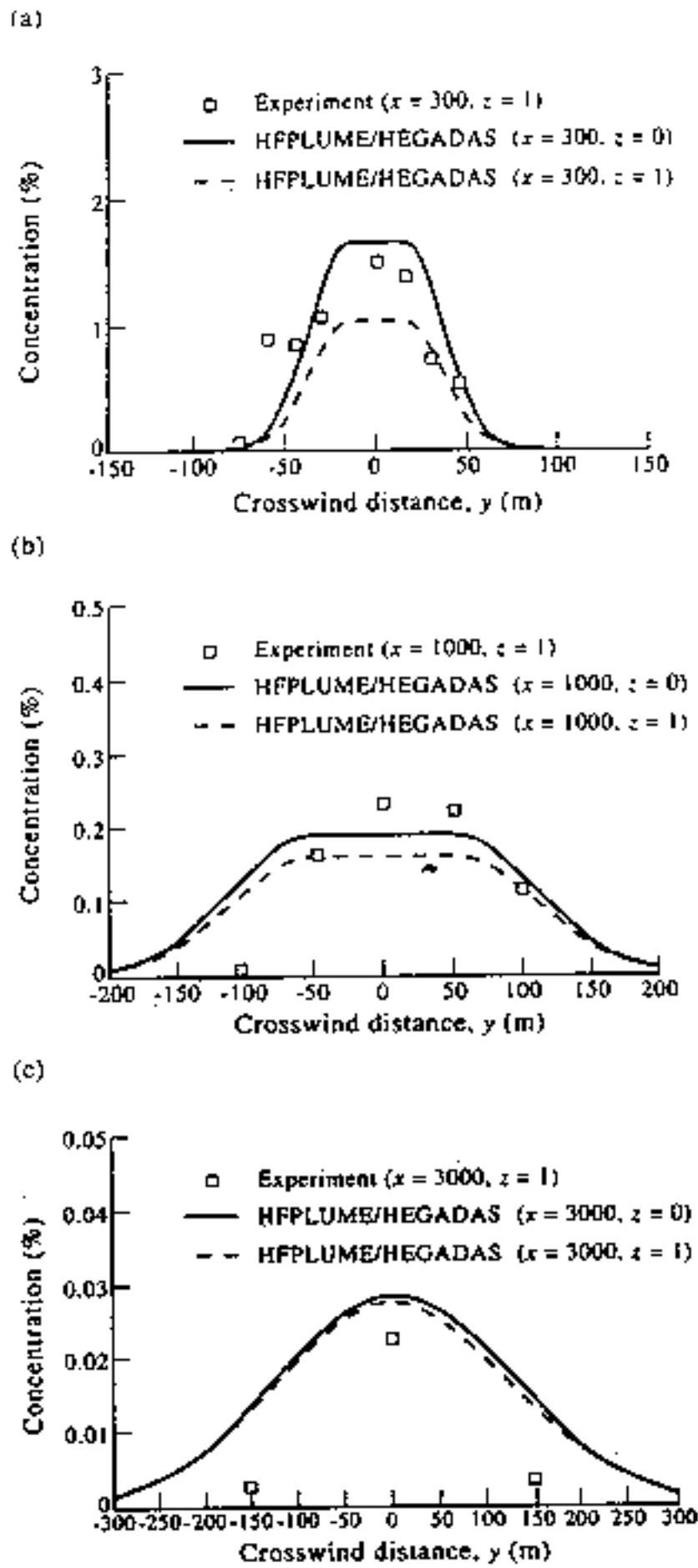


FIG. 15- HEGADAS predictions of crosswind ground-level concentration profile for Goldfish 3 experiment 3 at downwind distances of (a) 300 m, (b) 1000 m and (c) 3000 m

Appendix 7.A.A - Evaluation of ambient data

This Appendix describes the evaluation of the ambient data which are required in the dispersion calculations in HEGADAS.

WIND-SPEED PROFILE

The wind velocity in the atmospheric surface layer as a function of height z is taken from the following formula given by Businger (1973) and revised by Wieringa (1980),

$$u_a(z) = \frac{u_*}{\kappa} \cdot \left[\ln\left(\frac{z+z_R}{z_R}\right) - \Psi_m\left(\frac{z}{\lambda}\right) \right] \quad (\text{A.1})$$

where u_* is the ambient friction velocity, z_R the surface roughness, $\kappa = 0.41$ the Von Kármán constant and λ the Monin-Obukhov length; $\Psi_m(z/\lambda)$ is given by the following formulas for stable ($\lambda > 0$) and unstable ($\lambda < 0$) conditions:

$$\Psi_m\left(\frac{z}{\lambda}\right) = \begin{cases} -6.9 \cdot \frac{z}{\lambda} & (\lambda > 0) \\ 2 \cdot \ln[\frac{1}{2}(1+a)] + \ln[\frac{1}{2}(1+a^2)] - 2 \cdot \tan^{-1}(a) + \frac{1}{2}\pi & (\lambda < 0) \end{cases} \quad (\text{A.2})$$

with $a=(1 - 22 \cdot z/\lambda)^{1/4}$. Expression (A.1) is used directly in calculating u_* for given $u(z = z_0) = u_0$. Subsequently the exponent α in the HEGADAS power-law (2.1) is determined from the best fit with the ambient wind velocity (A.1). This matching is performed by means of least square fitting with a weighting function $w(z)=[1 + 10 \cdot z/z_0]^{-1}$, i.e. by minimising the functional

$$f(\alpha) = \int_0^{2z_0} w(z) \cdot [u_0 \cdot (z/z_0)^\alpha - u_a(z)]^2 dz \quad (\text{A.3})$$

over α .

TEMPERATURE AND DENSITY PROFILES

The potential temperature Θ (Kelvin) in the atmospheric surface layer as a function of height z is taken from the following formula given by Paulson (1970) and revised by Wieringa (1980),

$$\Theta - \Theta(z=0) = \frac{\Theta_*}{\kappa} \cdot \left[\ln\left(\frac{z+z_R}{z_R}\right) - \Psi_h\left(\frac{z}{\lambda}\right) \right] \quad (\text{A.4})$$

with

$$\Psi_h\left(\frac{z}{\lambda}\right) = \begin{cases} -9.2 \cdot \frac{z}{\lambda} & (\lambda > 0) \\ 2 \ln\left[\frac{1}{2} + \frac{1}{2} \cdot \left(1 - 13 \cdot \frac{z}{\lambda}\right)^{\frac{1}{2}}\right] & (\lambda < 0) \end{cases} \quad (\text{A.5})$$

$$\Theta_* = -\overline{u'_z T'} / u_* = u_*^2 T / [g\kappa\lambda] \quad (\text{A.6})$$

In the above formula T (Kelvin) is the ambient temperature at height z , T' is the turbulent fluctuation of T , u' is the turbulent fluctuation of u and the over-bar signifies an average over the turbulent fluctuations.

The potential temperature Θ is the temperature of the ambient air if it was brought adiabatically from the ambient pressure P to the pressure $P_0 = 1$ bar; Θ is related to the ambient temperature T by

$$\Theta = T \cdot (P_0 / P)^{R/C_p^a} = T \cdot (P_0 / P)^{0.2852} \quad (\text{A.7})$$

where $R = 8314.3$ J/K/kmole is the gas constant and $C_p^a = 29120$ J/K/kmole the specific heat of air. [Note. In HEGADAS the pressure P always equals 1 atmosphere, implying that $P_0 \approx P$ and $\Theta \approx T$].

Using equations (A.7) and (A.6) into (A.4) the following expression is obtained for the temperature profile in the atmospheric surface layer

$$T = T(z=0) / \left[1 - \frac{u_*^2}{\kappa^2 \cdot g \cdot \lambda \cdot (P_0 / P)^{0.2852}} \cdot \left[\ln\left(\frac{z+z_R}{z_R}\right) - \Psi_h\left(\frac{z}{\lambda}\right) \right] \right] \quad (\text{A.8})$$

Using the ideal-gas law $\rho_{\text{amb}} \cdot T = \rho_{\text{amb}}(z=0) \cdot T(z=0)$ leads to the following air-density profile,

$$\rho_{\text{amb}} = \rho_{\text{amb}}(z=0) \cdot \left[1 - \frac{u_*^2}{\kappa^2 \cdot g \cdot \lambda \cdot (P_0 / P)^{0.2852}} \cdot \left[\ln\left(\frac{z+z_R}{z_R}\right) - \Psi_h\left(\frac{z}{\lambda}\right) \right] \right] \quad (\text{A.9})$$

where the ground-level ambient density $\rho_{\text{amb}}(z=0)$ is found from the ideal-gas law,

$$\rho_{\text{amb}}(z = 0) = P \cdot m_{\text{amb}} / (R \cdot (T_a + 273.15)) \quad (\text{A.10})$$

with T_a (°C) the ambient temperature at ground level and m_{amb} the molecular weight of the humid air (kg/kmole).

MOLECULAR WEIGHT, WATER-VAPOUR PRESSURE AND ENTHALPY

The mole fraction of water in the ambient air is the ratio of the partial water-vapour pressure P_w^{amb} and the total ambient pressure P . Thus the molecular weight in equation (A.10) is defined by

$$m_{\text{amb}} = m_a \cdot [1 - P_w^{\text{amb}} / P] + m_w \cdot [P_w^{\text{amb}} / P] \quad (\text{A.11})$$

The partial water-vapour pressure P_w^{amb} is given by

$$P_w^{\text{amb}} = r_H \cdot P_v^w(T_a) \quad (\text{A.12})$$

with r_H the ambient humidity ($0 < r_H < 1$) and $P_v^w(T)$ the vapour pressure of water (atm) in 100% humid air at temperature T (°C).

In HEGADAS the formula $P_v(T)$ is taken from Lowe and Ficke (1974) for temperature T between 0 °C and 50 °C, and from an exponential formula for the vapour pressure of ice for $T < 0$,

$$P_v^w(T) = \begin{cases} a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4 + a_5 T^5 + a_6 T^6 & (0 < T < 50) \\ b_1 \exp(-b_2 / (T + 273.15)) & (T < 0) \end{cases} \quad (\text{A.13})$$

where the constants are given by $a_0=6.0279$, $a_1=4.3785 \cdot 10^{-1}$, $a_2=1.4102 \cdot 10^{-2}$, $a_3=2.6159 \cdot 10^{-4}$, $a_4=2.9916 \cdot 10^{-6}$, $a_5=2.0075 \cdot 10^{-8}$, $a_6=6.0566 \cdot 10^{-11}$, $b_1=3.452 \cdot 10^7$ and $b_2=6134$.

The enthalpy of the moist air (Joule/kmole of moist air) is given by

$$H_{\text{air}}^{\text{wet}} = \left\{ C_p^a \cdot (1 - P_w^{\text{amb}} / P) + C_p^{wv} \cdot (P_w^{\text{amb}} / P) \right\} \cdot (T_a - T^*)$$

where T^* is the reference temperature at which the enthalpy is taken to be zero; $T^*=25$ °C for the HF thermodynamics model (described in Chapter 2.B) and $T^*=0$ °C for the ideal-gas thermodynamics model (described in Chapter 2.A).

Appendix 7.A.B - Cross-wind diffusion effects

The derivation of the differential equation for the crosswind dispersion coefficient S_y is based on an empirical formula for the non-dense crosswind dispersion coefficient σ_y .

In HEGADAS-4 this formula is restricted to a power-law dependence of σ_y on the downwind distance x . Thus it does not allow for, for example, Briggs formula, which is more physically reasonable in the far field.

In this Appendix a generalised theoretical formulation for the evaluation of S_y is introduced. This formulation allows for any arbitrary empirical function $\sigma_y = \sigma_y(x)$, provided this function can be inverted to $x = x(\sigma_y)$.

In this section first the general formulation is given. Secondly the formulation is applied to Briggs formula.

BASIC EQUATIONS AND ASSUMPTIONS

The following basic equations and assumptions are adopted.

1. The crosswind concentration distribution used to describe passive dispersion is considered,

$$c = c_A \cdot \exp\left\{-\frac{1}{2} \cdot \left(\frac{y}{\sigma_y}\right)^2\right\} \quad (\text{B.1})$$

in which c_A is the centre-line concentration and σ_y is the crosswind dispersion coefficient.

2. The crosswind dispersion coefficient σ_y is assumed to be known as an invertible, empirical function of the downwind distance x ,

$$\sigma_y = \sigma_y^e(x) \quad (\text{B.2})$$

with the inverse

$$x = x^e(\sigma_y) \quad (\text{B.3})$$

3. The concentration profile (B.1) satisfies the simple two-dimensional diffusion equation

$$u_x \frac{\partial c}{\partial x} = \frac{\partial}{\partial y} \left(K_y \cdot \frac{\partial c}{\partial y} \right) \quad (\text{B.4})$$

in which u_x is the horizontal wind speed (independent of x and y) and K_y the crosswind diffusion coefficient. K_y is assumed to be proportional to u_x , with the proportional factor k_y being a (to be determined) function of the cloud half-width $W = (\pi/2)^{1/2} \cdot \sigma_y$,

$$K_y = u_x \cdot k_y = u_x \cdot k_y^e(W) \quad (\text{B.5})$$

REDUCED DIFFUSION EQUATION

Upon insertion of equations (B.1) and (B.5) the diffusion equation (B.4) reduces to

$$\frac{1}{c_A} \cdot \frac{\partial c_A}{\partial x} + \frac{y^2}{\sigma_y^3} \cdot \frac{\partial \sigma_y}{\partial x} = k_y^e(W) \cdot \left\{ \frac{y^2}{\sigma_y^4} - \frac{1}{\sigma_y^2} \right\} \quad (\text{B.6})$$

Since the above equation should apply for all y , we deduce the following two equations by equating powers of y ,

$$\frac{1}{c_A} \cdot \frac{\partial c_A}{\partial x} = -k_y^e(W) \cdot \frac{1}{\sigma_y^2} \quad (\text{B.7})$$

$$\sigma_y \cdot \frac{\partial \sigma_y}{\partial x} = k_y^e(W) \quad (\text{B.8})$$

The continuity equation,

$$\int_0^{\infty} u c \, dy = \text{constant} \quad (\text{B.9})$$

is by use of equation (B.1) easily seen to lead to $c_A \cdot \sigma_y \cdot u = \text{constant}$. Thus it can be shown that the system of equations (B.7), (B.8) is equivalent to the set of equations (B.9), (B.8). Hence equation (B.7) is not considered further, but attention is restricted to the differential equation (B.8) for σ_y .

By inserting equation (B.2) into equation (B.8), the dependence of k_y on the cloud half-width W can be determined,

$$k_y = k_y^e(W) = \sigma_y \cdot \frac{\partial \sigma_y^e}{\partial x} [x = x^e(\sigma_y)] \quad \text{with } \sigma_y = \sqrt{2/\pi} \cdot W \quad (\text{B.10})$$

EQUATIONS FOR THE CROSSWIND DISPERSION COEFFICIENT S_y

The derivation of equation (B.8) for the non-dense crosswind dispersion coefficient σ_y is based on the 'pure Gaussian' crosswind concentration profile (B.1).

In the HEGADAS concentration profile (2.2) the crosswind dispersion coefficient S_y corresponds to $2^{1/2} \cdot \sigma_y$; the concentration c is uniform in a middle part of half-width b and it exhibits Gaussian decay for $|y| > b$ only. Therefore in the calculation of S_y in HEGADAS-5 a generalisation of equation (B.8) is adopted for $b > 0$,

$$S_y \cdot \frac{\partial S_y}{\partial x} = 2 \cdot k_y^e(B_{\text{eff}}) \tag{B.11}$$

with $B_{\text{eff}} = b + W = b + 1/2 \sqrt{\pi} \cdot S_y$ being the effective half-width of the cloud.

The differential equation (B.11) is applied in HEGADAS for distances downwind of the pool with the middle part of the concentration profile $b > 0$. Let $x = x_t$ be the downwind distance at which b becomes 0. The following equation is adopted to evaluate S_y for $x > x_t$,

$$S_y(x) = 2^{1/2} \cdot \sigma_y^e(x + x_v) \quad (b = 0) \tag{B.12}$$

in which x_v is determined from

$$x_t + x_v = x^e \left(\sigma_y = 2^{-1/2} \cdot S_y(x_t) \right) \tag{B.13}$$

EXAMPLE: BRIGGS FORMULA FOR σ_y

Briggs formula and its inverse are given by

$$\sigma_y = \sigma_y^e(x) = \frac{\delta \cdot x}{\sqrt{1 + \gamma \cdot x}} \tag{B.14}$$

$$x = x^e(\sigma_y) = \frac{\sigma_y^2 \cdot \gamma}{2 \cdot \delta^2} \cdot \left\{ 1 + \sqrt{1 + \left(\frac{2 \cdot \delta}{\gamma \cdot \sigma_y} \right)^2} \right\}$$

Insertion of equation (B.14) into equation (B.8) leads to

$$k_y^e(W) = \frac{2 \cdot \delta^2}{\gamma} \cdot \{S^{-1} - S^{-2}\} \quad \text{with } S = S^e(W) = 1 + \sqrt{1 + 2 \cdot \pi \cdot \left(\frac{\delta}{\gamma \cdot W}\right)^2} \quad (\text{B.15})$$

For the option of Briggs formula, the equations for S_y now follow by insertion of equations (B.14), (B.15) into equations (B.11) and (B.12).

Appendix 7.A.C - Inclusion of heat and water-vapour transfer from substrate

This Appendix describes the inclusion into the HEGADAS model of heat and water-vapour transfer from the substrate to the vapour cloud. The user is referred to Section 5 in Appendix 3 of the HGSYSTEM version 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) for further (historical) details and experimental validation.

Heat transfer from the substrate to the gas cloud can be caused by both *natural* convection and *forced* convection. Heat and water vapour effects are included by adding a surface-heat transfer equation and a water-vapour equation for the two additional unknown quantities, i.e. the heat H_e added from the surface (Joule/kmole of mixture) and the water-vapour y_{w3} added from the surface (kmole/kmole of mixture).

C.1. Heat transfer from substrate

The heat transfer equation

$$\frac{1}{2 \cdot B_{\text{eff}}} \cdot \frac{d}{dx} [2 \cdot H_e \cdot B_{\text{eff}} \cdot H_{\text{eff}} \cdot u_{\text{eff}} / V_m] = Q_H \quad (\text{C.1})$$

describes the heat flux Q_H transferred from the substrate into the gas cloud (Joule/sec per unit of cloud width and per unit of cloud length).

The term between brackets in equation (C.1) represents the cloud heat flow through the plane $x = \text{constant}$ caused by pick-up of heat from the substrate (Joule/sec).

HEGADAS takes into account both the forced heat convection $Q_{H,f}$ and the natural heat convection $Q_{H,n}$.

For a substrate temperature T_s below the cloud temperature T_m the heat flux consists of only forced heat convection, while for $T_s > T_m$ the heat flux is chosen to be the maximum of forced and natural convection,

$$Q_H = \begin{cases} \max[Q_{H,n}, Q_{H,f}] & T_s > T_m \\ Q_{H,f} & T_s < T_m \end{cases} \quad (\text{C.2})$$

FORCED CONVECTION

Holman (1981) formulated the following expression for forced convection flux from the substrate to the vapour cloud,

$$Q_{H,f} = \frac{1}{2} \cdot \left(\frac{\alpha_T}{\nu} \right)^{2/3} \cdot C_f \cdot \rho_m \cdot c_p^m \cdot u \cdot (T_s - T_m) \quad (C.3)$$

where α_T is the thermal diffusivity (m²/s), ν the kinematic viscosity (m²/s), C_f the friction factor, ρ_m the mixture density (kg/m³), c_p^m the specific heat of the mixture (J/kg/K), u the gas velocity (m/s), and T_s and T_m the temperatures of substrate and mixture (°C).

For methane $\alpha_T/\nu = 1.35$; for other gases this ratio is only slightly different.

The friction factor $C_f = 2 (u_*/u)^2$, where u_* is the friction velocity (m/s).

For u we take the logarithmic wind velocity at 10 m height, u_{10} .

Thus expression (C.3) for forced convection heat flux can be rewritten as

$$Q_{H,f} = 1.22 \cdot \left(\frac{u_*^2}{u_{10}} \right)^2 \cdot \rho_m \cdot c_p^m \cdot (T_s - T_m) \quad (C.4)$$

where ρ_m , c_p^m , T_m are mixture properties at centre-line and ground level; c_p^m (J/kg/K) is given by

$$c_p^m = \frac{y_{pol} \cdot [(1 - \eta_w) \cdot C_p^{dp} + \eta_w \cdot C_p^{wv}] + (1 - y_{pol}) \cdot C_p^a}{y_{pol} \cdot [(1 - \eta_w) \cdot m_{dp} + \eta_w \cdot m_w] + (1 - y_{pol}) \cdot m_a} \quad (C.5)$$

with y_{pol} the ground-level centre-line mole fraction, C_p^{dp} , C_p^{wv} , C_p^a the molar specific heats (J/kmole/K) and m_{dp} , m_w , m_a (kg/kmole) the molecular weights of dry pollutant, water vapour and air, respectively.

NATURAL CONVECTION

McAdams (1954) formulated the following expression for natural convection flux from the substrate to the cold vapour cloud ($T_s > T_m$),

$$Q_{H,n} = 0.14 \cdot [\alpha_T^2 \cdot \zeta \cdot g \cdot (\rho \cdot c_p)^3 / \nu]^{1/2} \cdot (T_s - T_m)^{4/3} \quad (C.6)$$

where g is the gravitational acceleration (m/s²), c_p the specific heat (J/kg/K), ρ the density (kg/m³) and $\zeta = -\rho^{-1} \cdot (\partial\rho/\partial T)_p$.

Using the ideal gas law $P = R \cdot \rho \cdot T/m$ [P = pressure, T = temperature (K), R = gas constant, m = molecular weight], equation (C.6) can be rewritten as

$$Q_{H,n} = 0.14 \cdot g^{1/3} \cdot \frac{P}{R} \cdot \text{HEATGR} \cdot \left[\frac{(T_s - T_m)^2}{T} \right]^{2/3} \quad (\text{C.7})$$

with HEATGR defined by

$$\text{HEATGR} = \left[\left(\frac{\alpha_T}{v} \right)^2 \cdot \left(\frac{v}{T^2} \right) \cdot (m \cdot c_p)^3 \right]^{1/3} \quad (\text{C.8})$$

Strictly speaking the value of HEATGR in equation (C.8) should correspond to that of the mixture. Note that the natural convection heat flux given by equation (C.6) is only large if the substrate temperature is considerably lower than the mixture temperature, which can only occur if the concentration of the pollutant is very large. Therefore, for reasons of simplicity, the value of HEATGR is chosen to correspond to that for 100 % dry pollutant.

For methane, propane and air the value of the group equals 24, 29 and 20 $\text{m}^{-2/3} \text{s}^{-1/3} \text{K}^{-5/3} \text{kmole}^{-1} \text{J}$, respectively.

For T (Kelvin) in expression (C.6) we take the mean temperature $273.15 + (T_s + T_m)/2$.

In HEGADAS the pressure P is taken to be the standard atmospheric pressure (1 atm = 760 mm Hg).

C.2. Water-vapour transfer from substrate

The water-vapour transfer equation

$$\frac{1}{2 \cdot B_{\text{eff}}} \cdot \frac{d}{dx} [2 \cdot y_{w3} \cdot B_{\text{eff}} \cdot H_{\text{eff}} \cdot u_{\text{eff}} / V_m] = Q_{\text{wv}} \quad (\text{C.8})$$

describes the water-vapour flux Q_{wv} transferred from the substrate into the gas cloud (mole/sec per unit of cloud width and per unit of cloud length).

The term between brackets in equation (C.9) represents the molar flow of water through the plane $x = \text{constant}$ caused by pick-up of water-vapour from the substrate (mole/sec).

The mechanism by which condensation within the thermal boundary layer can increase the rate of evaporation from a liquid surface has been described by Rosner (1967). Using the theoretical approach of Rosner (1967), Colenbrander and Puttock (1984) derived the following expression for Q_{wv}

$$Q_{\text{wv}} = \begin{cases} \frac{1}{\Delta} \cdot \frac{P_v^w(T_s) - P_v^w(T_m)}{c_p^m \cdot T_s \cdot P} \cdot Q_H & T_s > T_m \\ 0 & T_s < T_m \end{cases} \quad (\text{C.10})$$

with $\Delta = 0.2$, P_v^w the vapour pressure of water given by equation (A.13) and c_p^m the specific heat of the mixture (Joule/kg/K) given by equation (C.5).

C.3. Effect of substrate water-vapour and heat transfer on entrainment

In the entrainment law (2.9),

$$\frac{1}{2 \cdot B_{\text{eff}}} \cdot \frac{d}{dx} [2 \cdot B_{\text{eff}} \cdot H_{\text{eff}} \cdot u_{\text{eff}} / V_m] = u_e (U_T) / V_0 + Q_{\text{wv}} \quad (\text{C.11})$$

the friction velocity u_* has been modified into u_T in order to take into account air entrainment caused by convective advents due to the temperature difference between the substrate and a cold vapour cloud.

Following Eidsvik (1980) u_T is taken to be

$$u_T = \sqrt{u_*^2 + (a \cdot w_*)^2} \quad \text{with } a = 0.2 \quad (\text{C.12})$$

with the velocity scale w_* a velocity scale for characterising the turbulence in a free convection layer,

$$w_* = \left[\frac{g \cdot Q_H \cdot H_{\text{eff}}}{T_m \cdot \rho_m \cdot C_{\text{pm}}} \right]^{1/3} \quad (\text{C.13})$$

The value $a = 0.2$ was found by comparing HEGADAS against experimental data.

Appendix 7.A.D - Evaluation of pollutant enthalpy

This Appendix discusses the evaluation of the pollutant enthalpy H_{pol} (Joule/mole of pollutant); H_{pol} is required as input parameter to the hydrogen fluoride (HF) and multi-compound two-phase aerosol thermodynamic models as discussed in Chapter 2.A and 2.B.

The pollutant enthalpy is determined by the pollutant temperature, the pollutant composition and the pollutant pressure. HEGADAS assumes the total pressure P always be equal to the ambient pressure, and therefore the pollutant pressure is assumed to be equal to the ambient pressure. Therefore for pressurised releases the pollutant temperature and the pollutant composition should correspond to the thermodynamic state immediately following depressurisation or (in the case of flashing) the post-flash state.

AEROSOL THERMODYNAMICS MODEL

For the aerosol thermodynamics model (Chapter 2.A), the pollutant consists of dry pollutant and water. In addition, the model allows for the inclusion of liquid water initially picked up from the substrate by the pollutant at the source.

Thus the pollutant is defined by the following input parameters.

- pollutant temperature, T_{pol} (°C)
- mole fraction of water originally in pollutant (at temperature T_{pol}), η_{wp}
- mole fraction of liquid water pick-up (at substrate temperature T_s), η_{ws}

Thus the total mole fraction of water in the pollutant equals $\eta_w = \eta_{wp} + \eta_{ws}$.

The water originally present in the pollutant may consist of vapour, liquid and/or ice. Let η_{wpv} , η_{wpl} , η_{wpi} be the mole fractions of original water vapour, liquid and ice, respectively, then $\eta_{wp} = \eta_{wpv} + \eta_{wpl} + \eta_{wpi}$ and

$$\eta_{wpv} = \min\left\{\eta_{wp}, (1 - \eta_{wp}) \cdot P_v^w(T_{pol}) / P\right\} \quad (D.1)$$

$$\eta_{wpl} = \eta_{wp} - \eta_{wpv}, \quad \eta_{wpi} = 0 \quad (T_{pol} > 0) \quad (D.2)$$

$$\eta_{wpi} = \eta_{wp} - \eta_{wpv}, \quad \eta_{wpl} = 0 \quad (T_{pol} < 0)$$

where the partial vapour pressure of water $P_v^w(T_{pol})$ is defined by equation (A.13).

The pollutant enthalpy equals the sum of the enthalpies for the dry pollutant, the water vapour, liquid and ice original present in the pollutant, and the water liquid pick-up

$$H_{pol} = (1 - \eta_w) \cdot C_p^{dp} \cdot T_{pol} + \eta_{wpv} \cdot C_p^{wv} \cdot T_{pol} + \eta_{wpl} \cdot (C_p^{wl} \cdot T_{pol} - H_{cond}^w) + \eta_{wpi} \cdot (C_p^{wi} \cdot T_{pol} - H_{fus}^w) + \eta_{ws} \cdot (C_p^{wl} \cdot T_s - H_{cond}^w) \quad (D.3)$$

Note. The HGSYSTEM 1.0 (or NOV90) version of HEGADAS may include liquid water pick-up, but does not allow water to be originally present in the pollutant ($\eta_{wp} = 0$).

HYDROGEN FLUORIDE THERMODYNAMICS MODEL

For the HF thermodynamics model (Chapter 2.B), the released pollutant consists of hydrogen fluoride (HF), an ideal gas (denoted by N-gas) and water. The model does not allow for the inclusion of liquid water pick-up from the substrate. Thus the thermodynamic state of the released pollutant is described by the following input parameters

- pollutant temperature, T_{pol} (°C)
- equivalent mole fraction of water, η_w (based on all HF in monomer state)
- equivalent mole fraction of N-gas, η_N (based on all HF in monomer state)

By applying the thermodynamic equations to the 100 % pollutant ($y_a = 0$, $T_m = T_{pol}$) the composition of the pollutant can be determined; see Chapter 2.B for details.

Subsequently the pollutant enthalpy is determined from the following formula (which is equal to equation (17) from Chapter 2.B)

$$\begin{aligned}
 H_{\text{pol}} = & E_{\text{pol}}^{\text{kin}} + \\
 & + \eta_{\text{HFL}} \cdot \{ C_p^{\text{HFL}} \cdot (T_{\text{pol}} - T^*) - H_{\text{cond}}^{\text{HF}} \} + \\
 & + \{ \eta_{\text{N}} \cdot \{ C_p^{\text{N}} \cdot (T_{\text{pol}} - T^*) \} + \\
 & + [\eta_{\text{w}} - (1 - x_{\text{pol}}) \cdot L_{\text{pol}}] C_p^{\text{wv}} \cdot (T_{\text{pol}} - T^*) + \\
 & + [\eta_{\text{HF}} - \eta_{\text{HFL}} - x_{\text{pol}} \cdot L_{\text{pol}}] \cdot \{ H_{\text{pol}}^{\Delta\text{HF}} + C_p^{\text{HFV}} \cdot (T_{\text{pol}} - T^*) \} + \\
 & - x_{\text{pol}} \cdot L_{\text{pol}} \cdot \{ H_{\text{cond}}^{\text{HF}} + H_{\text{mix}} \} + \\
 & - (1 - x_{\text{pol}}) \cdot L_{\text{pol}} \cdot H_{\text{cond}}^{\text{w}} + \\
 & + L_{\text{pol}} \cdot \{ C_p^{\text{fog}}(x_{\text{pol}}, T_{\text{pol}}) \cdot (T_{\text{pol}} - T^*) \}
 \end{aligned} \tag{D.4}$$

Note. The HGSYSTEM 1.0 (or NOV90) version of HEGADAS does not allow for presence of N-gas and/or water in the pollutant, and η_{w} , η_{N} , L_{pol} are set equal to zero in equation (D.4).

Appendix 7.A.E - Observer position and observer speed

In order to express the observer dispersion data as a function of position and time, a formula needs to be provided for the position of each observer as a function of time. Ideally the observers should move with the average transport velocity u_{eff} of the vapour molecules (effective cloud speed) defined by equation (2.6).

At a given location x the value of S_z and accordingly u_{eff} differ from observer to observer and consequently some observers may overtake others. Therefore a simplified formula will be introduced which is a function of x only.

The simplified formula is assumed to be based on the two-dimensional case: no cross-wind spreading effects ($B_{\text{eff}} = \text{constant}$), a constant Richardson number Ri_* , neglect of heat and water vapour transfer from the substrate ($Q_{\text{wv}} = 0$, $Q_{\text{H}} = 0$, $u_{\text{T}} = u_*$) and a constant mixture volume V_{m} . For this case the entrainment equation (2.9) can be solved analytically for $M_{\text{eff}}^{\text{mol}}$, and subsequent use of equation (2.7) yields the following formula for S_z ,

$$S_z = S_z(x) = z_0 \cdot \left\{ \frac{\kappa \cdot \beta \cdot u_* \cdot V_{\text{m}} \cdot (x - x_0)}{\Gamma((1 + \alpha) / \beta) \cdot \Phi(Ri_*) \cdot u_0 \cdot V_0 \cdot z_0} \right\}^{1/(1+\alpha)} \quad (\text{E.1})$$

with x_0 an integration constant.

Insertion of equation (E.1) into equation (2.6) for the effective cloud speed yields the following formula for the observer speed as a function of x ,

$$u^{\text{obs}} = u^{\text{obs}}(x) = C_0 \cdot \left[\frac{(x - x_0)}{z_0} \right]^{\alpha/(1+\alpha)} \quad (\text{E.2})$$

with

$$C_0 = \frac{\Gamma((1 + \alpha) / \beta)}{\Gamma(1 / \beta)} \cdot u_0 \cdot \left\{ \frac{\kappa \cdot \beta \cdot u_* \cdot V_{\text{m}}}{\Gamma((1 + \alpha) / \beta) \cdot \Phi(Ri_*) \cdot u_0 \cdot V_0} \right\}^{\alpha/(1+\alpha)} \quad (\text{E.3})$$

By integrating equation (E.2) to time the following formula for the observer position can be derived

$$x(t) = x_0 + z_0 \cdot \left\{ \left(\frac{x_{\text{st}}^{\text{obs}} - x_0}{z_0} \right)^{1/(1+\alpha)} + \frac{C_0}{z_0 \cdot (1 + \alpha)} \cdot (t - t_{\text{st}}^{\text{obs}}) \right\}^{1+\alpha} \quad (\text{E.4})$$

with x_{st}^{obs} the downwind distance and t_{st}^{obs} the time, at which the observer is released (where $x(t=t_{st}^{obs}) = x_{st}^{obs}$).

It now remains to evaluate the constants x_0 and C_0 in the above equations.

DISPERSION FROM GROUND-LEVEL POOL

The observers are released at $x = x_{st}^{obs} = -R_{max}$, where R_{max} is the maximum radius of the secondary source $R(t)$. The following two assumptions are now made:

1. At the point of release the observer speed equals zero,

$$u^{obs}(x = x_{st}^{obs} = -R_{max}) = 0 \quad (E.5)$$

2. Let R_m be the radius of the secondary source when the take-up rate $\pi R^2 Q$ is maximum, and let $S_z(x = \frac{1}{2}\pi^{1/2}R_m; E = \pi R^2 Q, B = \frac{1}{2}\pi^{1/2}R_m, L = \pi^{1/2}R_m)$ be the value of S_z at the downwind edge of a steady-state square source of strength $E = \pi R^2 Q$, half-width $B = \frac{1}{2}\pi^{1/2}R_m$ and length $L = \pi^{1/2}R_m$.

The observer velocity at $x = \frac{1}{2}\pi^{1/2}R_m$ is then taken to be the effective cloud speed for this steady source at $x = \frac{1}{2}\pi^{1/2}R_m$.

Using equation (2.6) it is found that

$$u^{obs}(x = \frac{1}{2}\sqrt{\pi} \cdot R_m) = u_0 \cdot \frac{\Gamma((1+\alpha)/\beta)}{\Gamma(1/\beta)} \cdot \left[\frac{S_z(x = \frac{1}{2}\sqrt{\pi} \cdot R_m)}{z_0} \right]^\alpha \quad (E.6)$$

Imposing the assumptions (E.5) and (E.6) upon (E.2) leads to

$$x_0 = -R_{max} \quad (E.7)$$

$$C_0 = u_0 \cdot \frac{\Gamma((1+\alpha)/\beta)}{\Gamma(1/\beta)} \cdot \left[\frac{S_z(x = \frac{1}{2}\sqrt{\pi} \cdot R_m)}{z_0} \right]^\alpha \cdot \left[\frac{\frac{1}{2}\sqrt{\pi} \cdot R_m + R_{max}}{z_0} \right]^{-\alpha/(1+\alpha)} \quad (E.8)$$

DISPERSION FROM VERTICAL TRANSITION PLANE (BREAKPOINT)

The observers are released at the transition plane (breakpoint) $x = x_{st}^{obs} = x_{br}$. The constant x_0 is first determined by matching at $x = x_{br}$ equation (E.2) for the observer speed against a typical value of u_{eff} derived from the breakpoint data. Subsequently the constant C_0 is determined.

The effective cloud speed u_{eff} can be set from equation (2.6) and the value of S_z calculated at the breakpoint $x = x_{\text{br}}$. However the latter value for S_z varies from observer to observer. Therefore to arrive at a fixed value, the value of S_z is chosen to correspond to the breakpoint value $S_z^{\text{br}}(t_m)$ at the time t_m when the gas-flow rate $E_{\text{br}}(t)$ is maximum. The value for u_{eff} thus obtained from equation (2.6) is now assumed to be the value of the observer speed at x_{br} ,

$$u^{\text{obs}}(x_{\text{br}}) = u_0 \cdot \frac{\Gamma((1+\alpha)/\beta)}{\Gamma(1/\beta)} \cdot \left\{ \frac{S_z^{\text{br}}(t_m)}{z_0} \right\}^{\alpha} \quad (\text{E.9})$$

Thus by inserting equation (E.9) into (E.12) it follows that

$$x_0 = x_{\text{br}} - z_0 \cdot \left\{ \frac{u_0 \cdot \Gamma((1+\alpha)/\beta)}{C_0 \cdot \Gamma(1/\beta)} \right\}^{(1+\alpha)/\alpha} \cdot \left\{ \frac{S_z^{\text{br}}(t_m)}{z_0} \right\}^{1+\alpha} \quad (\text{E.10})$$

The constant C_0 is assumed to be defined by equation (E.3) with $V_m = V_0$ and with Ri_* assumed to be value of the Richardson number at the breakpoint at time t_m , i.e. $Ri_* = Ri_*^{\text{br}}(t_m)$.

Appendix 7.A.F - Cloud shape correction for downwind gravity spreading

In low wind velocities HEGADAS simulations of time-dependent spills show considerable gravitational spreading of high density vapour clouds (e.g. propane) after the initial slumping of the vapour blanket.

Since the HEGADAS model allows for gravitational spreading in the crosswind direction only, the calculated crosswind dimensions are too large and the dimensions in wind direction too small.

As cloud shape becomes a parameter of increasing importance in more refined hazard assessment methods, a cloud-shape-correction routine has been designed for the time-dependent HEGADAS computer program. The basic consideration for this correction is that the gravitational spreading velocity should be the same in all directions. The HEGADAS model generates a cloud at a specified point of time consisting of elements (observer intervals) with calculated height, length, width and concentration. These elements retain their length while travelling downwind and spreading in the crosswind direction. Leaving height and concentration unchanged, as well as the product of length and width of each element, the width is reduced and the length increased in such a way that the amount of spreading in the downwind direction of the cloud as a whole equals the spreading in the crosswind direction. A subroutine of the HEGADAS time-dependent computer program contains the mathematical formulation of this correction which is described below.

Let L_c be the calculated cloud length and W_c the cloud width at a specified point at time t , and let W_0 be the initial cloud width.

The cloud width and length is now corrected in such a way that the spreading S in downwind direction equals the spreading in crosswind direction. This means, if L_c^{cor} and W_c^{cor} are defined to be the corrected length and width, that $L_c^{cor} = L_c + S$ and $W_c^{cor} = W_0 + S$.

Conservation of cloud surface area then requires

$$L_c^{cor} \cdot W_c^{cor} = L_c \cdot W_c \quad \text{or} \quad (L_c^* + S^*) \cdot (1 + S^*) = L_c^* \cdot W_c^* \quad (\text{F.1})$$

with $L_c^* = L_c/W_0$, $W_c^* = W_c/W_0$ and $S^* = S/W_0$.

Given L_c^* and W_c^* , equation (F.1) can be solved for S^* :

$$S^* = -\frac{1}{2}(1 + L_c^*) + \frac{1}{2}\sqrt{(1 + L_c^*)^2 + 4 \cdot L_c^* \cdot (W_c^* - 1)} \quad (\text{F.2})$$

so that

$$L_c^{\text{corr}} / L_c = (L_c^* + S^*) / L_c^* \quad (\text{F.3})$$

$$W_c^{\text{cor}} / W_c = (1 + S^*) / W_c^* \quad (\text{F.4})$$

Consider now an element i (observer interval) of the cloud with length Δx^i and half-width B_{eff}^i . The element i remains fixed at its location but its length and width are corrected in analogy to the above equations,

$$\Delta x^{\text{cor},i} / \Delta x^i = (L_c^* + S^{*i}) / L_c^* \quad (\text{F.5})$$

$$B_{\text{eff}}^{\text{cor},i} / B_{\text{eff}}^i = (1 + S^{*i}) / W_c^{*i} \quad (\text{F.6})$$

with

$$S^{*i} = -\frac{1}{2}(1 + L_c^*) + \frac{1}{2}\sqrt{(1 + L_c^*)^2 + 4 \cdot L_c^* \cdot (W_c^{*i} - 1)} \quad (\text{F.7})$$

$$W_c^{*i} = B_{\text{eff}}^i / B_{\text{eff},0}^i \quad (\text{F.8})$$

with $B_{\text{eff},0}^i$ the initial effective cloud half-width for element i .

Again, these correction formulae satisfy the essential condition of conservation of element surface area: $\Delta x^{\text{cor},i} \cdot B_{\text{eff}}^{\text{cor},i} = \Delta x^i \cdot B_{\text{eff}}^i$.

Let t_j be the j^{th} output time specified by the user. Let observer i be the observer released at time $t_{\text{st}}^i = t_{\text{st}} + i \cdot \Delta t_{\text{obs}}$ ($i = 1, 2, \dots$), and let x_j^i be the downwind position of observer i at time t_j .

Let the observers i_j^L, i_j^R ($i_j^L > i_j^R$) be the observers which at time t_j see some gas ($y_{\text{pol},j}^i > 0$) and which are located most upwind ('left') and downwind ('right'), respectively.

Let observer i_j^M be the observer with the maximum concentration (maximum value for $y_{\text{pol},j}^i$; if the maximum is found in more than one element, the one located furthest from the source is chosen).

The corrected downwind positions and crosswind dispersion data at time k for observer i are denoted by $x_i^{\text{cor},k}, b_i^{\text{cor},k}$ and $S_{y,i}^{\text{cor},k}$.

The algorithm for the cloud-shape correction adopted in HEGADAS is described below for the cases of a ground-level pool and a transition plane, consecutively.

DISPERSION FROM GROUND-LEVEL POOL

1. Set the initial cloud width W_0 equal to the maximum diameter of the gas blanket above the source. Set the initial half-width $B_{\text{eff},0}^i$ for observer i ($i = 1,2,\dots$) equal to the half-width B_i of the source seen by the observer (see equation (3.12)).

2. Loop over the specified output times t_j ($j = 1,2,\dots$):
 - a Determine observers $IL = i_j^L$, $IR = i_j^R$, $IM = i_j^M$ ($IL > IM > IR$).
Set cloud length $L_c = (x_{IR}^k - x_{IL}^k)$. Set $L_c^* = L_c/W_0$.

 - b Loop over the observers $i = IL, IL-1, \dots, IR+1, IR$:
 - If $b_j^i > 0$ set $W_c^{*i} = B_{\text{eff},j}^i/B_{\text{eff},0}^i$ else $W_c^{*i} = 1$ (see equation (F.8)).
 - Set S^{*i} from equation (F.7).
 - Correct crosswind dispersion parameters for observer i by applying equation (F.6) to both the middle part and the Gaussian flanks of the crosswind concentration profile:
 $b_j^{\text{cor},i}/b_j^i = S_{y,j}^{\text{cor},i}/S_{y,j}^i = (1+S^{*i})/W_c^{*i}$.
 - This implies that no correction is applied since $W_c^{*i} = 1$, $S^{*i} = 0$ if $b_j^i = 0$.

 - c The cloud shape correction is started at observer IM :
 - Fix downwind location of observer IM : $x_j^{\text{cor},IM} = x_j^{IM}$.
 - Apply cloud shape correction (F.5) consecutively for observers $i = IM-1, IM-2, \dots, IL$ to set corrected observer positions downwind of x_j^{IM} :
$$x_j^{\text{cor},i} = x_j^{\text{cor},i+1} + (x_j^i - x_j^{i+1}) \cdot (L_c^* + S^{*i})/L_c^*$$
 - Apply cloud shape correction (F.5) consecutively for observers $i = IM+1, IM+2, \dots, IR$ to set corrected observer positions upwind of x_j^{IM} :
$$x_j^{\text{cor},i} = x_j^{\text{cor},i-1} - (x_j^{i-1} - x_j^i) \cdot (L_c^* + S^{*i})/L_c^*$$

DISPERSION FROM VERTICAL TRANSITION PLANE (BREAKPOINT)

1. Set the initial cloud width W_0 equal to the maximum cloud width specified at the breakpoint. Set the initial effective half-width $B_{\text{eff},0}^i$ for observer i ($i = 1,2,\dots$) equal to the effective cloud half-width $B_{\text{eff}}^{\text{br}}(t_{st}^i)$ seen by the observer at the transition plane.

2. Loop over the specified output times t_j ($j = 1,2,\dots$):
 - a see point 2a for case of dispersion from ground-level pool

b see point 2b for case of dispersion from ground-level pool

c The cloud shape correction is started at the most upwind observer IL :

- Fix downwind location of observer IL : $x_j^{cor,IL} = x_j^{IL}$.
- Apply cloud shape correction (F.5) consecutively for observers $i = IL-1, IL-2, \dots, IR$ to set corrected observer positions downwind of x_j^{IL} :

$$x_j^{cor,i} = x_j^{cor,i+1} + (x_j^i - x_j^{i+1}) \cdot (L_c^* + S^{*i}) / L_c^*$$

If the output time t_k equals the time $i \cdot \Delta t$ at which the present observer i is released at the breakpoint, it follows from the above that $W^{*i} = 1$, $S^{*i} = 0$, $IL = i$.

Thus the crosswind dispersion parameters b , S_y and the downwind position x remain unchanged. This implies that the conditions at the breakpoint x_{br} remain satisfied during the cloud shape correction.

7.B. PLUME SPREAD AND AIR ENTRAINMENT FORMULATION

7.B.1. Introduction

This chapter describes changes made to the HEGADAS model following a review of the treatment of lateral plume growth for dense clouds. The changes apply to the transition region where density effects become less important and turbulence increasingly determines the rate of plume spread. A concomitant change to the HEGADAS entrainment assumptions is described.

7.B.2. Plume spread and entrainment in HEGADAS

As described in section 7.A.2.3. the HEGADAS model assumes that a dense gas cloud passes through *three stages of lateral cloud growth*.

Initially the cloud spreads as a *gravity current* at a rate given by equation 7.A.2.12a (equation 2.12a in chapter 7.A.). The gravity current then *collapses* and the plume spreads slowly according to equation 7.A.2.12c which is developed assuming that flow is still driven by gravitational effects. Lastly, lateral plume growth is determined by *turbulent diffusion* and is described by empirical correlations based on field experiments, equation 7.A.2.13*.

The gravity current and slow spreading zones are sharply delineated by a phenomenon which is named *gravity current collapse*. The possibility of gravity current collapse was suggested by a comparison (Roberts (1990)) of HEGADAS predictions against some wind tunnel experiments carried out by Petersen and Ratcliff (1989). This comparison showed that the measured plume widths were much narrower than those predicted by HEGADAS. Petersen and Ratcliff (1989) themselves obtained similar results when comparing their data with other dense gas models (SLAB, DEGADIS). Conversely, the dense gas models *underpredicted* gas concentrations.

A semi-empirical correlation was developed for the onset of collapse using the wind tunnel data together with results from some lock-exchange experiments carried out by Linden and Simpson (1988) to investigate frontogenesis. Frontogenesis is one process by which gravity currents form in the atmosphere and ocean and is characterised by the sharpening of horizontal density gradients and increasing vertical density stratification. Linden and Simpson (1988) showed that mechanical stirring which destroyed the vertical density stratification in a gravity current caused the propagation speed to drop. It was hypothesised by us that this could be the

cause of gravity current collapse in the wind tunnel when boundary layer turbulence provides the required vertical mixing. The correlation developed by us is given by equation 7.A.2.12b.

The mechanism that triggers the gravity current collapse is still not clearly understood. We hypothesised that some external event destroyed the leading edge of the current, converting the flow into one driven by a horizontal hydrostatic pressure gradient similar to that characterising the lock exchange experiments. This uncertainty is reflected in the empiricism of equation 7.A.2.12b, which also lacks a clear physical interpretation. We now recognise that this semi-empirical formula (7.A.2.12b) can be rewritten as:

$$\frac{u_e \cdot B_{\text{eff}}}{u_g \cdot H_{\text{eff}}} \geq \text{constant} \quad (1)$$

where we have substituted the gravity spreading velocity, $u_g = \frac{dB_{\text{eff}}}{dt}$, (equation 7.A.2.12a) and entrainment velocity, u_e , (equation 7.A.2.10), in place of the explicit dependencies on the Richardson numbers (Ri and Ri_*).

The left hand side of equation (1) is a measure of the rate of volumetric addition of air (per unit downwind distance) into a cloud of height H_{eff} and width B_{eff} divided by the rate of volumetric growth of the cloud due to lateral gravity spread. When this ratio exceeds unity, the flow of air mixed into the top of the cloud exceeds the increase in cloud volume due to lateral expansion and the cloud height must increase, significantly changing the vertical distribution of dense gas. This process erodes the vertical density stratification within the body of the cloud that is needed to maintain the gravity current.

The criterion (1) is therefore a measure of the destruction of the internal vertical structure of the gravity current by mixing driven by the external turbulence. This is a much more robust and physically plausible interpretation of gravity current collapse than that made previously in which we required a "trigger" to destroy the leading edge.

We have since carried out a series of independent wind-tunnel experiments (Roberts and Hall, 1994), which have confirmed the measurements of Petersen and Ratcliff and established that equation 7.A.2.12b offers an adequate measure of the maximum cloud size attained by gravity spreading. This is therefore retained in the HEGADAS model.

The expression for the rate of cloud spread after gravity current collapse, equation 7.A.2.12c, derives from the analysis of flow due to a horizontal hydrostatic pressure gradient. It is numerically dependent on the wind-tunnel results of Petersen and Ratcliff through the

constant C_D and, when applied to full scale problems the cloud spreading velocity (dB_{eff}/dt) appears overly small compared to characteristic turbulence velocities (u_*). Equation 7.A.2.12c assumes that the flow is due to gravitational influences, and while this is true to the original HEGADAS assumptions, it has the incorrect asymptotic behaviour in the far-field, tending to vanish as $Ri \rightarrow 0$ whereas we should require that:

$$\frac{dB_{\text{eff}}}{dx} \rightarrow \frac{d\sigma_y}{dx} \quad \text{as } Ri \rightarrow 0 \quad (2)$$

On both of these grounds the formulation is unsatisfactory; equation 7.A.2.12c must have a limited range of applicability and should be replaced. The replacement must satisfy the initial conditions that dB_{eff}/dx be small after gravity current collapse, asymptote to $d\sigma_y/dx$ for large x and permit development of the HEGADAS concentration profile as discussed below. The formulation must give similar numerical results to 7.A.2.12c when used for wind-tunnel calculations.

We note that, for the wind-tunnel experiments used to set the value of C_D , dB_{eff}/dx was everywhere numerically similar to the values of $d\sigma_y/dx$ measured for neutrally buoyant (that is, $Ri = 0$) releases.

HEGADAS assumes that an initially top-hat concentration profile evolves into a Gaussian profile as set out in equations 7.A.2.2. The edges of the Gaussian plume are of width, S_y , and are assumed to grow according to equation 7.A.2.13. This equation is derived from the cross-wind diffusion equation and assumes a mixing-length eddy diffusivity based on plume width as described in section 7.A.2.3. The properties of this formulation are such that, when the edges join, the plume is entirely Gaussian, $S_y = \sqrt{2} \cdot \sigma_y$ and satisfies the input correlation for σ_y .

The development of the Gaussian edges in HEGADAS is assumed *not* to contribute to the overall plume width (B_{eff}). This is a reasonable assumption if the growth rate of the edges is very small compared to the overall lateral growth rate of the plume, but is inappropriate when turbulent diffusion is the faster process. This instance must arise if the plume is ever to reach a fully Gaussian cross-sectional profile. We therefore now assume that the overall plume width grows in sympathy with the thickness of the mixing layer which forms the Gaussian edge of the plume, and neglect the contribution of the lateral hydrostatic pressure gradient (equation 7A.2.12c).

We take

$$B_{\text{eff}} \cdot \frac{dB_{\text{eff}}}{dx} = 2 \cdot k_y^*(S_y) \quad (3)$$

by analogy with the model for S_y and with the function k_y^* chosen so that when $B_{\text{eff}} = \frac{1}{2} \sqrt{\pi} \cdot S_y$ equation (3) becomes identical to equation 7.A.2.13.

This formulation represents a solution to the diffusion equation with a diffusivity based on the mixing layer thickness S_y . It has the correct asymptotic behaviour and ensures that B_{eff} always increases more slowly than S_y so that the HEGADAS concentration profile always evolves to the Gaussian shape. When the input correlation for $\sigma_y(x)$ takes wind-tunnel values the numerical value of (3) is similar to that of equation 7.A.2.12c.

The changed assumptions about the mechanism of plume spread post gravity current collapse require some amendment of the HEGADAS entrainment model.

HEGADAS originally assumed that while the cloud width was prescribed by a gravity spreading equation the only active entrainment process is by mixing through the top of the cloud, equation 7.A.2.9.

This is an *exact* assumption for a gravity current in which there is no mixing across the leading edge and the cloud has a top-hat concentration profile. It is a *poor* assumption when turbulent diffusion acts to broaden the cloud and air is entrained by both lateral and vertical mixing. This was recognised in HEGADAS and was represented by a change in the entrainment equation from:

$$\frac{1}{2 \cdot B_{\text{eff}}} \cdot \frac{d}{dx} [2 \cdot B_{\text{eff}} \cdot H_{\text{eff}} \cdot u_{\text{eff}} / V_m] = u_e(u_T) / V_0 + Q_{\text{wv}} \quad 7.A.2.9$$

which states that the total molar addition of air to the cloud takes place through the upper surface to:

$$\frac{d}{dx} [H_{\text{eff}} \cdot u_{\text{eff}} / V_m] = u_e(u_T) / V_0 + Q_{\text{wv}} \quad 7.A.2.9^*$$

which represents the molar addition by entrainment per unit width of cloud.

It is implicitly assumed that the increase in the total molar flow due to the increase in plume width with distance arise through separate entrainment processes associated with lateral plume growth.

This change in equation formulation was imposed at the end of the 'gravity' regime which was marked by the attainment of a Gaussian concentration profile.

We previously discussed the evolution of the HEGADAS concentration profile, and identified that it was incorrect to neglect the contribution of lateral diffusion to plume width growth when lateral diffusion was faster than gravity spreading - as it must be for the HEGADAS profile to become Gaussian. In the same way it is incorrect to neglect the entrainment contribution from lateral diffusion. We therefore limit the applicability of equation 7.A.2.9 above to the region where the plume spreads as a gravity current and apply equation 7.A.2.9* everywhere downwind of the point of gravity current collapse.

We note that we could also implement this change by specifying the *additional entrainment* that arises through lateral mixing as a source term in equation 7.A.2.9. We could go further and develop a closure for the plume width B_{eff} based on the entrainment description as an alternative to equation (1).

7.B.3. Illustration of model changes

The effects of these changes to HEGADAS are have been illustrated using two examples which differ in the input correlation for $\sigma_y(x)$. The magnitude of $\sigma_y(x)$ has been doubled by changing the input averaging time. This changes the distance over which the cloud is 'gravity' dominated as well as the width of the cloud in the far-field.

Calculations have been carried out using the original HEGADAS-4 (no gravity current collapse) and HEGADAS-5 (as available in HGSYSTEM version 1.0) to illustrate the effect of the changes. The results shown in figure 1 use an instantaneous averaging time and in figure 2 a ten minute (600 s) averaging time.

Figure 1 compares predictions of plume width (1a) and of centreline concentration (1b) for the original HEGADAS-4 model, for HEGADAS-5 as supplied with HGSYSTEM 1.0 and for the revised model (as available in HGSYSTEM version 3.0) described here.

Figure 1 highlights the very large difference in plume width predictions arising from the assumption of gravity current collapse in HEGADAS-5. The model revisions give slightly greater plume width predictions than HEGADAS-5 near to the slope discontinuity that marks the start of the Gaussian profile, but matches smoothly both at the point of gravity current collapse and in the far-field. The concentration predictions show similar behaviour. The

original model (HEGADAS-4) predicts significantly lower concentrations in the near field than HEGADAS-5. The new model gives intermediate concentrations and smoothes the slope discontinuity in the HEGADAS-5 predictions.

Figure 2 shows similar calculations, but now for an averaging time of 600 s. Here the input correlation for σ_y has a larger value so that the point at which the HEGADAS profile becomes Gaussian in the original HEGADAS-4 and HEGADAS-5 models moves upstream. Again the new model gives slightly greater plume-widths and slightly lower concentrations than HEGADAS-5. The difference between the new model and the original HEGADAS-4 predictions is also reduced.

We note that figure 2 shows quite clearly that the slope discontinuities in width and concentration existed in the formulation of the original HEGADAS model and were not artefacts of the HEGADAS-5 (HGSYSTEM version 1.0) version.

7.B.4. References

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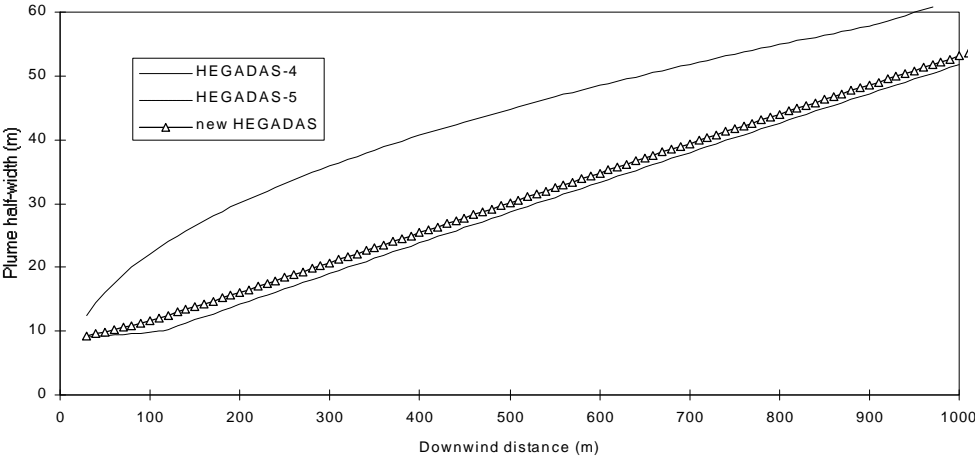


Figure 1a. Comparison of plume half-widths for an instantaneous release.

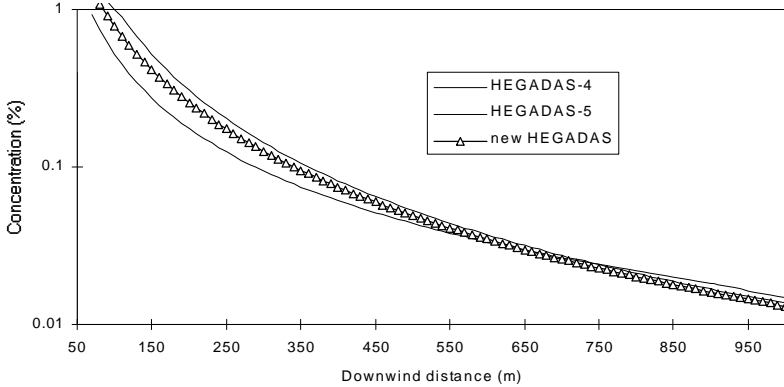


Figure 1b. Comparison of concentration profiles for an instantaneous release.

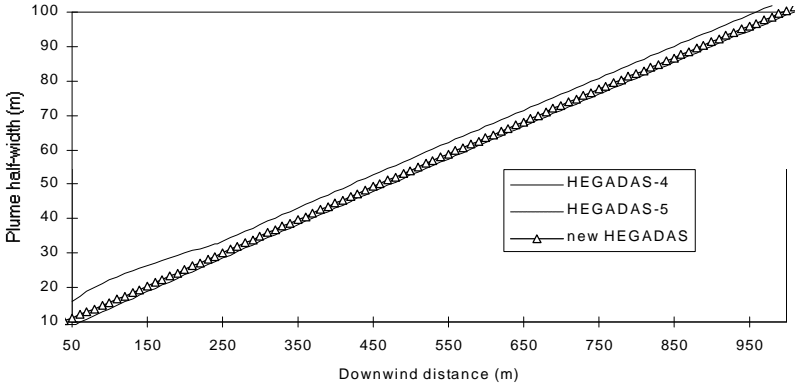


Figure 2a. Comparison of plume half-widths for a 600 s release.

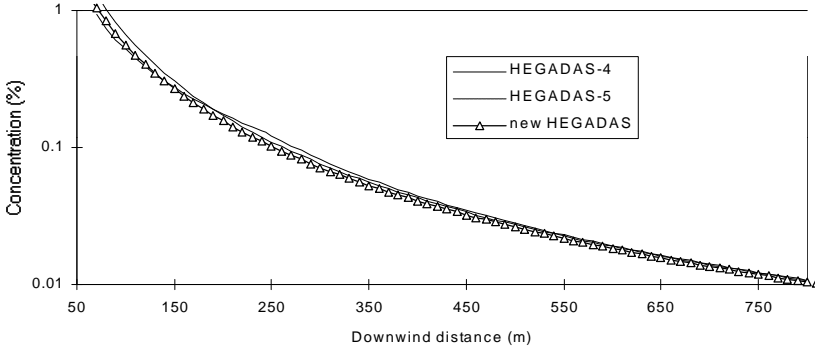


Figure 2b. Comparison of concentration profiles for a 600 s release.

7.C. NEW OPTIONS FOR THE HEGADAS MODEL

This Chapter discusses new options added to the HEGADAS model compared to the descriptions as given in Chapter 7.A. Most options apply to HEGADAS-T only and are intended to make the use of this complicated model more straightforward.

The options are only available in the HEGADAS model as supplied with *version 3.0* of HGSYSTEM and not in the 1.0 version.

7.C.1. Automated output times in HEGADAS-T

7.C.1.1. Introduction

When using the HEGADAS-T model to calculate transient dispersion phenomena, the user can study the results using a concentration versus downwind distance plot. This plot will contain separate concentration versus distance profiles for each requested output time.

These output times are chosen correctly if concentration values for intermediate output times can be calculated accurately enough using linear interpolation.

It usually takes considerable trial and error to find a proper set of output times for a given dispersion scenario. To avoid this time-consuming approach, an algorithm to calculate output times automatically has been developed. Using this algorithm will increase the total run-time per HEGADAS-T calculation, but the user will obtain useful extra information on the quality of the used set of output times. It is envisaged that the user spends a few runs to determine a proper set of output times using the algorithm. Once a suitable set of output times has been found, there is no need to use the algorithm again for similar scenarios.

For *every* run of HEGADAS-T (using the automatic output time algorithm or not), the program prints out information in the report file concerning the quality of the set of output times used. Based on this information, the user can decide to use the automatic generation of output times or not. Note that this information is calculated after taking the effects of along-wind diffusion and cloud shape correction into account.

The option to let HEGADAS-T calculate output times automatically, is available for all three HEGADAS-T scenarios: evaporating pool, post-AEROPLUME run and for a post-HEGABOX run. These cases had to be treated differently in the code.

Before the normal dispersion calculations are performed for all output times and for the required number of observers, the output time algorithm first performs dispersion calculations for a limited set of observers and for a set of three successive output times.

On the basis of the results thus obtained the algorithm decides whether the step between the output times can be increased or not. Then dispersion calculations for the next set of three output times are performed, again for the observer subset.

This process continues until a user-specified last output time has been reached.

The automatic output time algorithm is similar to the observer algorithm as discussed in section 3.2 of Chapter 7.A.

7.C.1.2. Algorithm

In the current implementation of the automatic output time algorithm, a subset of six (6) observers is taken.

For a post-HEGABOX run the total number of observers is always 21. The subset observer indices are 1, 5, 9, 13, 17 and 21. For the other two scenarios a maximum of 161 observers can be used. The subset indices are taken as 1, 33, 65, 97, 129 and 161.

For the selected observer subset, dispersion calculations are performed *only* for the current set of three (consecutive) output times, denoted by t_1 , t_2 and t_3 . These calculations do not take along-wind diffusion and a cloud shape correction into account.

The initial set of three output times is always taken as $t_1 = t_{\text{first}}$, $t_2 = t_{\text{first}} + \Delta t$ and $t_3 = t_{\text{first}} + 2 \cdot \Delta t$. Here t_{first} is the user-specified first output time and Δt is the output time step.

As a result for every observer i in the subset a value of the ground level concentration for the output times t_1 , t_2 and t_3 is found. Let these concentrations be denoted by $c(i,t)$.

To judge whether the time step between two consecutive output times can be increased, the 'exact' value of $c(i,t_2)$ is compared with a value based on *linear interpolation* between the t_1 value $c(i,t_1)$ and the t_3 value $c(i,t_3)$. This is done for all observers i in the subset.

Let $c_{\text{inter}}(i,t_2)$ denote this interpolated value then

$$c_{\text{inter}}(i, t_2) = c(i, t_1) + (t_2 - t_1) \cdot \frac{c(i, t_3) - c(i, t_1)}{t_3 - t_1} \quad (1)$$

Per observer, an error $E(i)$ is being defined as the (absolute) difference between the value found using linear interpolation, $c_{\text{inter}}(i,t_2)$, and the 'exact' value, $c(i,t_2)$, normalised by the maximum concentration for that output time. In other words, $E(i)$ is defined as

$$E(i) = \frac{|c_{inter}(i, t_2) - c(i, t_2)|}{c_{max}(t_2)} \quad (2)$$

where $c_{max}(t_2)$ is defined as

$$c_{max}(t_2) = \max_{i \text{ in subset}} c(i, t_2) \quad (3)$$

Now a *mean error* MEANERR is defined as the average of the $E(i)$'s over all N observers in the subset, where the currently used value of N is 6.

$$MEANERR = \frac{1}{N} \cdot \sum_{i=1}^N E(i) \quad (4)$$

A *maximum error* MAXERR can also be defined as

$$MAXERR = \max_{i \text{ in subset}} E(i) \quad (5)$$

Using the same error measure as used in the (existing) algorithm for automated observer release, the mean absolute error MEANERR is taken to be the criterion for the automatic output time calculation. This reflects the idea that the *overall curve* should be represented accurately enough.

If MEANERR is *greater* than a pre-set tolerance ϵ , then the algorithm proceeds with a new set of three output times, where new t_1 value is the old t_2 value and the new t_2 value is the old t_3 value. The new value for t_3 is simply $t_3 + \Delta t$. The dispersion calculations are then repeated for these new output times and a new value for MEANERR is calculated.

If MEANERR is *less* than the tolerance ϵ , then the output time step Δt is increased by multiplying it with a pre-set factor α . Thus effectively the distance between all output times coming *after* the current ones, is increased. The next set of three output times is found as above. The new value for t_3 is again $t_3 + \Delta t$, but now the *new* (increased) value for Δt is used.

If MEANERR is greater than $3 \cdot \epsilon$, then a warning message is printed by the program. In this case the user might consider choosing a smaller (initial) value for Δt , a smaller value for α or a larger value for t_{first} (the latter implies that the first cloud print output location will be further away from the source).

For a post-HEGABOX run the number of observers is fixed (21). Therefore with increasing t_{last} , the distance between observers will increase, leading to larger errors. In this case choosing a smaller value for t_{last} will decrease the value of MEANERR.

If the value of MAXERR is too large (larger than $(N-1) \cdot \epsilon$), then a warning message is printed. Thus the algorithm cycles through sets of three output times, each time judging whether it is possible to increase the time step to be used in the *next* set of output times..

This process stops when either a maximum number of output times has been found (currently this maximum is 20) or when a new output time t_3 exceeds a user-specified last output time t_{last} . The last output time is always taken to be exactly equal to t_{last} , if the maximum number of output times has not been reached yet.

Because of the way the algorithm works, the value of t_{last} must always at least be equal to $t_{\text{first}} + 2 \cdot \Delta t$. The HEGADAS-T program checks for this and modifies t_{last} if necessary.

For a post-AEROPLUME run or a post-HEGABOX run, t_{first} must always exceed the time at which the transition takes place. The code again checks for this.

After all calculation have been completed by HEGADAS-T, a final check is made where per output time the values of MEANERR and MAXERR are recalculated but now for *all* observers used. The largest value of MEANERR and MAXERR for all used output times are then printed in the report file to serve as a check for the user on the quality of the output time choice.

This information is *always* printed, also when the automatic output times algorithm was not used. Thus the user can decide to use the algorithm in subsequent runs.

7.C.1.3. Implementation

In the HEGADAS-T input file the user can either specify explicit output times using the CALC input block or he can use the option of automatic output times generation using the new input block AUTOTIM .

The user must always specify either the CALC or the AUTOTIM input block, but not both. The HEGADAS-T program will check that precisely one of these two input blocks has been specified.

The AUTOTIM input block has two *mandatory* input parameters, TFIRST and TLAST. TFIRST is the first output time and TLAST the last one.

The value of TLAST should be at least equal to $TFIRST + 2 \cdot DTMIN$, where DTMIN is the initial step Δt between output times.

The user can optionally specify DTMIN. The default value for DTMIN is 20.0 seconds.

It is also optional to specify OTEPS, the tolerance ϵ used in the algorithm, or OTFACT, the multiplication factor α used in the algorithm. The default value for OTEPS is 0.05 (or 5 %) and the default value for OTFACT is 1.50.

Monitoring and warning messages are printed both to the screen and the report file.

On the basis of this information the user should check whether his current set of parameters for the Δt algorithm is satisfactory or not.

7.C.2. Automatic downwind stepsize in HEGADAS-T

7.C.2.1. Introduction

When using the HEGADAS-T program, dispersion data is reported per output time for a series of equidistant downwind distances. Let Δx be the stepsize between the downwind reporting distances. For small output times, the value of Δx should be small enough to represent the concentration profile correctly. For larger output times, the downwind distances will be larger and larger values for Δx will be sufficient to give an accurate plot of concentration as a function of downwind distance.

In the steady-state program HEGADAS-S it is possible to let the value of Δx become larger with increasing values of downwind distance x . In the transient program HEGADAS-T the value of Δx used to be constant per program run.

A new algorithm implemented in HEGADAS-T to increase the value of Δx for larger output times, while still maintaining a reliable representation of the concentration profile, will be discussed now.

The option to let HEGADAS-T increase the value of Δx automatically is available for all three HEGADAS-T scenarios: evaporating pool, post-AEROPLUME run and for a post-HEGABOX run.

The general idea behind the Δx algorithm is that the value of Δx can be increased if the use of linear interpolation between given ground level concentrations at given downwind distances gives a reliable estimate of the concentration values at intermediate downwind distances.

7.C.2.2. Algorithm

For a given output time, the ground level concentrations are given at a series of N equidistant downwind distances $x_{\text{first}}, x_{\text{first}} + \Delta x, x_{\text{first}} + 2 \cdot \Delta x, \dots, x_{\text{last}} = x_{\text{first}} + (N-1) \cdot \Delta x$, where N is an integer number.

The values of x_{first} and x_{last} are determined by the HEGADAS-T program and are chosen in such a way that concentrations outside the interval $[x_{\text{first}}, x_{\text{last}}]$ are negligible for the current output time.

Consider all N-2 sets of three consecutive equidistant downwind distances x_1, x_2 and x_3 , with $x_1 = x_{\text{first}} + (i-1) \cdot \Delta x, x_2 = x_{\text{first}} + i \cdot \Delta x$ and $x_3 = x_{\text{first}} + (i+1) \cdot \Delta x$, for $i = 1, 2, \dots, N-2$.

Let the ground level concentration at downwind distance x be denoted by $c(x)$. To check whether the stepsize Δx can be increased for the *next* output time, the values of $c(x)$ for all the sets of three values of x are being considered. A given set of three consecutive x values is indexed by $i = 1, 2, \dots, N-2$, the three concentrations per set are denoted by $c(i, x_1), c(i, x_2)$ and $c(i, x_3)$.

The 'exact' value of $c(i, x_2)$ is compared with a value based on *linear interpolation* between the value at distances x_1 and x_3 . Let $c_{\text{inter}}(i, x_2)$ denote this interpolated value then

$$c_{\text{inter}}(i, x_2) = c(i, x_1) + (x_2 - x_1) \cdot \frac{c(i, x_3) - c(i, x_1)}{x_3 - x_1} \quad (6)$$

Per set of three x values, an error $E(i)$ is defined as the absolute difference between the interpolated value $c_{\text{inter}}(i, x_2)$ and the 'exact' value $c(i, x_2)$, normalised by the maximum concentration occurring at x_2 . The expression for $E(i)$ is thus

$$E(i) = \frac{|c_{\text{inter}}(i, x_2) - c(i, x_2)|}{c_{\text{max}}(x_2)} \quad (7)$$

with $c_{\text{max}}(x_2)$ defined as

$$c_{\text{max}}(x_2) = \max_{i=1, \dots, N-2} c(i, x_2) \quad (8)$$

After calculating the values of $E(i)$ for all $i = 1, 2, \dots, N-2$, several error measures can be calculated. The *maximum error* MAXERR for the current output time is defined as

$$\text{MAXERR} = \max_{i=1, \dots, N-2} E(i) \quad (9)$$

The *mean error* MEANERR is defined as

$$\text{MEANERR} = \frac{1}{N-2} \cdot \sum_{i=1}^{N-2} E(i) \quad (10)$$

Using the same error measure as in the automatic output time algorithm and as in the automated observer release algorithm, the mean absolute error MEANERR is taken as the criterion for the automatic downwind stepsize algorithm.

Calculations with HEGADAS-T have shown that even for quite smooth concentration curves, with a low MEANERR value, it can happen that $E(i)$ is quite large for a very few i -values. Usually points with a high value for $E(i)$ are at the front and at the end of the gas cloud, where large relative changes in concentration occur because of the steep 'flanks'.

An illustration of this is given in Figure 1, where an example $c(i,x)$ curve has been plotted and relative errors have been given for some i -values. In Figure 1, the mean relative error is 0.015, which is quite low, but the maximum relative error is 0.165, which is 11 times higher. The value for Δx in this example is 0.10 m and N is 48. The maximum concentration used to normalise the errors is 0.0709 kg/m³ in this example.

This example supports the choice to base the criterion to increase the value of Δx on the value of MEANERR. The value of MAXERR is printed out in the report file to enable the user to monitor the development of the gas cloud profile.

If MEANERR is *greater* than a pre-set tolerance ϵ , then for the next output time the value of the stepsize Δx is *not* changed.

If MEANERR is *less* than the tolerance ϵ , then the value of Δx is multiplied by a pre-set factor α . This new value of Δx will be used in the printout of dispersion data for the *next* output time.

If MEANERR is greater than $3 \cdot \epsilon$, then a warning message is printed by the program. In this case the user might consider choosing a smaller initial value for Δx , a smaller value for α or a larger value for the first output time (the latter implies that the first cloud print output location will be further away from the source).

If the value of MAXERR is found to be very large (larger than $(N-1) \cdot \epsilon$), then a warning message is printed in the report file.

The HEGADAS-T code will only use the Δx algorithm if, for the current output time, there are at least five consecutive downwind distances where dispersion data is being reported.

7.C.2.3. Implementation

The HEGADAS-T input parameters involved in the Δx algorithm have been added to the already available CLOUD input block.

The parameter XSTEP, default value 10 metre, should now be interpreted as the *initial* value of Δx . The new parameters XSEPS and XSFACT are the tolerance ϵ and the multiplication factor α respectively. The default value for XSEPS is 0.05.

The default value for XSFACT is 1.0, which indicates to HEGADAS-T that the Δx algorithm is *not* to be used. Thus if the user wants to use the Δx algorithm it is *mandatory* to specify a value for XSFACT not equal to 1.0. A reasonable value for XSFACT when using the algorithm is 1.5.

Monitoring and warning messages are printed to the report file only. On the basis of this information the user should check whether his current set of parameters for the Δx algorithm is satisfactory or not.

Per output time, HEGADAS-T saves the series of reported downwind distances x and ground level concentrations $c(x)$ in two arrays with size ALLMAX. The current value of ALLMAX is 100. For very small (initial) values of Δx , this array size might be too small. Only the first ALLMAX values of x and $c(x)$ are then used in the Δx algorithm. The HEGADAS-T program will print out a warning when ALLMAX is too small and the user can then consider increasing the size of ALLMAX in the HEGADAS-T Fortran code (routine CLOUDC).

7.C.3. Surface roughness breakpoints in HEGADAS-T

7.C.3.1. Introduction

The steady-state heavy gas dispersion program HEGADAS-S allows the user to specify several so-called *breakpoints* using the TRANSIT input block.

A *full* breakpoint occurs when a transition from AEROPLUME to HEGADAS-S is being made. Data from AEROPLUME is made available to HEGADAS-S using the TRANSIT and TIMEDATA input blocks as written to the link file.

The user can also specify a *partial* breakpoint using the TRANSIT block, if at a certain downwind distance he wants to change the value of some variable. The description in the User's Manual of the TRANSIT input block, lists the variables that can currently be reset at a partial breakpoint.

One of these variables is the surface roughness z_r . Thus currently in HEGADAS-S the user can specify a change in surface roughness at a specified downwind distance. This can be done for up to 20 downwind distances; in other words the TRANSIT block can be specified up to 20 times to define a partial breakpoint.

In the transient heavy gas program HEGADAS-T a full breakpoint formulation is available, which is identical to the HEGADAS-S full breakpoint option.

Also for HEGADAS-T, an out-of-date (HEGADAS-4) partial breakpoint formulation was available in HGSYSTEM 1.0, which was not advocated to be used. However, this formulation did not allow the user to change the surface roughness.

To facilitate users wanting to change the surface roughness at downwind locations, a new surface roughness breakpoint formulation has been implemented and at the same time the out-of-date HEGADAS-4 breakpoint formulation has been removed from the HEGADAS code.

HEGADAS-T now allows the user to set multiple breakpoints (up to 20) where the surface roughness can be reset. *Only* the surface roughness can be changed at these breakpoints.

Please note that the provision of this facility is *not* expected to give a simple means of performing accurate simulations of dispersion over a change in surface roughness. See section 7.6.2. in the HGSYSTEM 1.0 Technical Reference Manual for comments on the original HEGADAS-S implementation of surface roughness breakpoints.

The actual implementation of this new roughness breakpoint is not a straightforward task due to the complexity of the transient HEGADAS version.

Although different implementations are necessary for the different HEGADAS-T scenarios, the surface roughness breakpoint option is available for all three HEGADAS-T scenarios: the standard evaporating pool case , a post-AEROPLUME run and a post-HEGABOX run.

7.C.3.2. Algorithm

For every observer used in the HEGADAS-T calculations, a HEGADAS-S dispersion calculation is needed to obtain the total transient dispersion behaviour. Within the steady-state calculation per observer, the change in surface roughness z_r is taken into account in the same way as in HEGADAS-S.

To avoid serious complications, the distances travelled by each observer are calculated using constants based on the *initial* value of z_r .

For values of z_r less than about 0.5 m and for all atmospheric stability classes, a sensitivity study has shown that this simplification has little effect on the calculated observer distances. It is recommended only to use z_r values less than 0.5 m, when specifying a surface roughness breakpoint in HEGADAS-T.

When the surface roughness changes, a large number of other parameters have to be updated. One of these is the Monin-Obukhov length which is a function of surface roughness and stability class.

Normally the HEGADAS code will calculate the Monin-Obukhov length itself and in this case it will be updated automatically when a surface roughness change occurs. Note however, that if the user has *explicitly specified* a certain value for the Monin-Obukhov length, by using the MONIN keyword in the DISP input block, then this value will *not* be updated when the surface roughness changes.

The implementation of the surface roughness breakpoint option in HEGADAS-T has been tested by comparing HEGADAS-T individual observer results with HEGADAS-S results. In these comparisons the cloud correction algorithm was not used.

It should be noted that the post-processor POSTHT in HGSYSTEM version 3.0 uses a constant ALPHA to calculate off-centre, above-ground level concentrations. ALPHA depends on z_r . Although in the dispersion calculations in HEGADAS-T the value of ALPHA is updated when z_r changes, in POSTHT the *initial* value of ALPHA is used. Centre-line, ground level concentrations are computed correctly in POSTHT even when z_r changes.

7.C.3.3. Implementation

To use the new surface roughness breakpoint, the user can specify the TRANSIT input block up to 20 times. In this block the DISTTS parameter is mandatory; this parameter specifies the downwind distance at which the breakpoint occurs.

If the user *only* specifies the DISTTS parameter, then HEGADAS-T will treat the breakpoint as a *full* breakpoint and additional information must be specified in the TIMEDATA input block. A full breakpoint can only be specified *once*. See the User's Manual for details.

To define a *surface roughness* (partial) breakpoint, in addition to the DISTTS parameter, the ZRS parameter must also be given in the TRANSIT block. The ZRS parameter specifies the new value of the surface roughness.

As an example, assume that the user has specified an initial surface roughness of 0.01 m. In other words, the DISP input block contains the line

$$ZR = 0.01$$

Now assume that the user wants to change the value of the surface roughness to 0.1 m at a downwind distance of 100 m. The following lines should then be added to the input file

TRANSIT

$$DISTTS = 100$$

$$ZRS = 0.1$$

Thus in the HEGADAS-T dispersion calculations, for downwind distances less than 100 m, the used value for z_r is 0.01 m and for downwind distances greater than 100 m, the used value of z_r is 0.1 m.

7.C.4. Other new options

7.C.4.1. Volumetric concentrations in CLOUD input block

In the CLOUD input block, three concentrations could be specified. CAMIN is the ground-level centre-line concentration (in kg/m³) at which calculations will stop. CU and CL are upper and lower concentration limits (in kg/m³) used in contouring and cumulative cloud data.

Three new parameters, COMIN, CUV and CLV, have been added to the CLOUD block, these being the volumetric counterparts of the existing parameters CAMIN, CU and CL.

COMIN (in vol-%) has the same function as CAMIN.

CUV and **CLV** (both in vol-%) have the same function as CU and CL.

Normally the user should either specify CAMIN or COMIN. If CAMIN and COMIN are both specified, COMIN will be used. If neither CAMIN nor COMIN is specified, then COMIN will be used with a default value. Normally the user should specify either CU or CUV. If CU and CUV are both specified then CUV will be used. If neither CU nor CUV is specified, then CUV will be used with a default value.

Whenever CUV (vol-%) has a value, a value of CU (kg/m³) is calculated for use in contouring and cloud contents calculations. The calculated value of CU is

$$CU = \frac{CUV}{100} \cdot \frac{MM}{22.4} \cdot \frac{273.15}{273.15 + TAP} \quad (11)$$

where MM is the molar mass of the dry pollutant and TAP is the ambient temperature at reference height. Note that this method only gives an *approximate* conversion of the vol-% value CUV to a kg/m³ value CU but in the far field it will be quite appropriate.

Also note that the only situation where this conversion will be *not* be used, is if CU, *but not* CUV, has been specified by the user.

The CL and CLV parameters are treated analogously to the CU and CUV parameters.

It is not necessary to specify only vol-% or only kg/m³ values. All combinations of three out of the six parameters are allowed.

The default value for CUV is 2.0 vol-%, for COMIN and CLV the default is 0.1 vol-%. Defaults for CAMIN, CU and CL are no longer relevant: if they are not user-specified, the vol-% counterpart will be used.

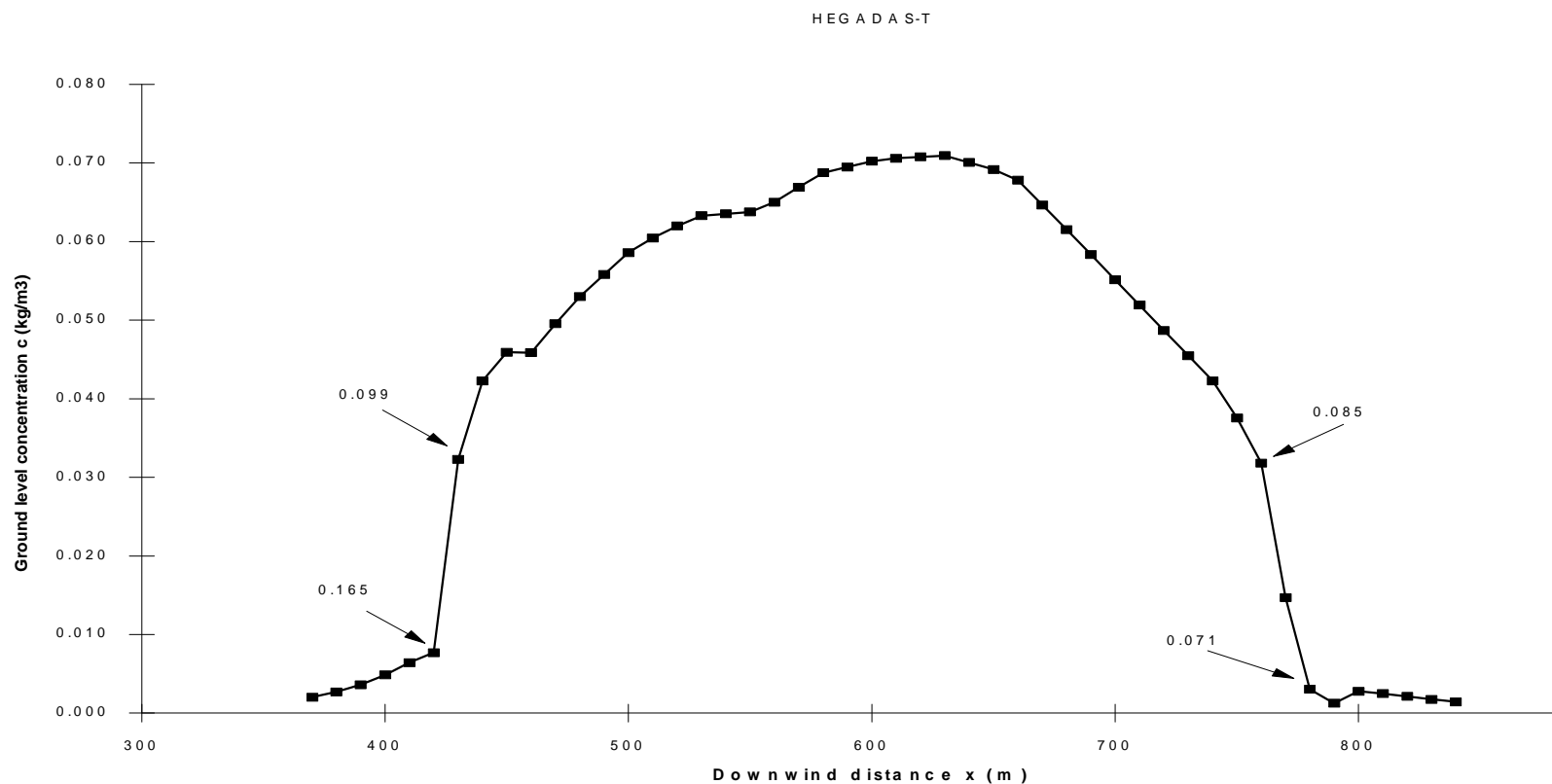


Figure 7.C.1. Example of HEGADAS-T concentration profile. Mean error is 0.015, maximum error is 0.165. Labels indicate individual errors. Maximum concentration 0.0709 kg/m³. Step size Δx is 0.10 m.