6. THE PGPLUME MODEL FOR FAR-FIELD DISPERSION

CONTENTS

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6.1. Introduction

The influence upon plume dispersion of release conditions and of complex reaction dynamics decreases with increasing downwind distance, and becomes negligible when compared with ambient turbulence in the far-field. Inasmuch as the formulation of ambient turbulence within the HGSYSTEM plume models (AEROPLUME/HFPLUME for HGSYSTEM version 3.0 and PLUME/HFPLUME for HGSYSTEM version 1.0) is rather uncertain, it is inappropriate to extrapolate these plume models far downwind of release.

For the regime of passive advection considerable (empirical) success has been obtained by means of a Gaussian plume/'image'-plume model. Local concentrations are prescribed in terms of horizontal and vertical standard deviations, each expressed as a function of distance downwind of the source. Atmosphere stability is described by the familiar Pasquill/Gifford classes 'A' through 'F;'. The correlations apply properly to extended and level terrain (Pasquill 1961, Gifford 1975). More recent developments allow correction of the standard correlations for surface roughness (Hanna 1982), for concentration averaging time (plume meander) (Hanna, Briggs and Hosker 1982), for release duration (Blewitt, Yohn, and Ermak 1987), and for the influence of the nearby ground (Pasquill 1976).

We may choose either to modify the entrainment function within the HGSYSTEM plume models, or else to link these models to the well established Pasquill/Gifford Gaussian plume model.
Modifications might incorporate the Pasquill/Gifford standard deviations into the entrainment function (Bloom 1980; Petersen and Cermak 1980); or else represent surface layer structure implied by observation and Monin-Obukhov similarity (Ooms 1972; Schatzmann 1978; Disselhorst 1984) in such a way as to reproduce observed far-field behaviour.

The choice of method is governed by computational efficiency and by the need to ensure *accurate* reproduction of well-known far-field effects. We link HFPLUME to a Pasquill/Gifford model by asymptotic matching, in which a virtual source for a Pasquill/Gifford model is located by requiring the continuity of mass, momentum, and energy fluxes between near and far-field descriptions at a (given) matching plane. Subsequent dispersion is then obtained by function evaluation, rather than by the numerical solution of a set of ordinary differential equations. The matching procedures are broadly analogous to those proposed in the context of heavy gas dispersion by Raj and Morris (1987).

The HGSYSTEM model which can describe the far field passive dispersion is called PGPLUME. All HGSYSTEM plume models (AEROPLUME and HFPLUME in version 3.0 of HGSYSTEM) can make a transition (link) to PGPLUME if appropriate.

6.2. Far-field Dispersion: Pasquill/Gifford Models

The dispersion of a trace contaminant from a ground or an elevated point source over flat homogeneous terrain is well described by an (essentially empirical) plume/'image'-plume model of the general form (Stern, Boubel, Turner and Fox 1984; Hanna 1982; Briggs and Hosker 1982):

Point-local concentration

$$c(Dx,y,z)/c_* = y(y,z;s_y,s_z,z_{PG}) \qquad (1)$$

$$c_* = dm/dt_0/[2\ p\ u_¥\ s_y\ s_z] \qquad (2)$$

where $y(y,z;s_y,s_z,z_{PG}) = \exp(-y^2/(2s_y^{\,2}))\ [\exp(-(z - z_{PG})^2/(2s_z^{\,2})) + \exp(-(z + z_{PG})^2/(2s_z^{\,2}))]$ (3)

and $s_y,s_z = (s_v,s_z)(Dx = x_{PG} - \langle x\rangle, z_{PG};t,z_{cm},z_r)$

z ³ 0; Dx ³ 0

-¥ < y < ¥

z_{cm}, z_{PG}, s_y, s_z ³ 0

Notation: Dx displacement downwind of a (virtual) point-source of pollutant mass-flux dm/dt_0 at co-ordinates (x_{PG},0,z_{PG}); c_* 'centre-line' mass-concentration at displacement Dx; (x_{PG} + Dx,y,z) co-ordinates of a general point within the Pasquill/Gifford plume a distance z above ground, and a (horizontal) distance y off-axis; (s_y,s_z) standard deviations in horizontal and vertical directions (m); $u_¥$ mean wind-speed (m/s); z_{cm} plume centre-of-mass (centroid) height (m).

Pollutant is *advected* at the (vertical-mean) wind-speed $u_¥$. Cross-wind dispersion is described by vertical and horizontal standard deviations s_z and s_y respectively. Each standard deviation depends on the atmosphere stability (class), distance downwind of the source (Gifford 1976), the chosen concentration averaging time (Pasquill 1976), Hanna 1982), the surface roughness (Hanna and Briggs 1984), and the mean plume (centroid) 'height' (Pasquill 1976).

The standard Pasquill/Gifford standard deviations based upon a (reference) surface roughness z_r^{PG} = 3cm, ground-level source, and a (reference) averaging time t_{PG} = 10 minutes (Hanna, Briggs and Hosker 1982) were given graphically for distances less than some 10-50 km downwind of release. These correlations were given numerical form by Turner and Busse (1973), who proposed for s_y^{PG} the dimensioned form (Stern, Boubel, Turner and Fox 1984),

Horizontal Standard Deviation

$$s_y^{PG} = 465.116\ (Dx/10^3)\ \tan(\theta\ p/180) \qquad (4)$$

$\theta(Dx,PG) =$	$24.167 - 2.5334 \ln(Dx/10^3)$	PG = 'A'	
	$18.333 - 1.8096 \ln(Dx/10^3)$	PG = 'B'	
	$12.500 - 1.0857 \ln(Dx/10^3)$	PG = 'C'	(5)
	$8.3333 - 0.72382 \ln(Dx/10^3)$	PG = 'D'	
	$6.2500 - 0.54287 \ln(Dx/10^3)$	PG = 'E'	
	$4.1667 - 0.36191 \ln(Dx/10^3)$	PG = 'F'	

with 0 £ Dx < 100 km and PG = {'A','B','C','D','E','F'}

Notation: Dx downwind distance (m); PG Pasquill/Gifford stability class; s_y^{PG} standard (Pasquill/Gifford) horizontal standard deviation (m).

In addition the vertical standard deviation s_z^{PG} is assigned for each stability class a piece-wise power-law form (Turner and Busse 1973; Stern, Boubel, Turner and Fox 1984).

Vertical Standard Deviation

$s_z^{'A'} =$	$122.80Dx^{0.9447}$	Dx < 100 m	$s_z^{'B'} =$	$90.673Dx^{0.93198}$	Dx < 200 m
	$158.08Dx^{1.0542}$	100 m £ Dx £ 150 m		$98.483Dx^{0.98332}$	200 m £ Dx £ 400 m
	$170.22Dx^{1.0932}$	150 m < Dx £ 200 m		$109.30Dx^{1.09710}$	400 m £ Dx £ 35 km
	$179.52Dx^{1.1262}$	200 m < Dx £ 250 m		5000m	Dx > 35 km
	$217.41Dx^{1.2644}$	250 m < Dx £ 300 m	$s_z^{'C'} =$	$61.141Dx^{0.91465}$	0 m < Dx
	$258.89Dx^{1.4094}$	300 m < Dx £ 400 m	$s_z^{'D'} =$	$34.459Dx^{0.86974}$	Dx < 300 m
	$346.75Dx^{1.7283}$	400 m < Dx £ 500 m		$32.093Dx^{0.81066}$	300 m < Dx £ 1 km
	$453.85Dx^{2.1166}$	500 m < Dx £ 3.11 km		$32.093Dx^{0.64403}$	1 km < Dx £ 3 km
	5000	Dx > 3.11 km		$33.504Dx^{0.60486}$	3 km < Dx £ 10 km
				$36.650Dx^{0.56589}$	10 km < Dx £ 30 km
				$44.053Dx^{0.51179}$	Dx > 30 km

where the σ's are in m.

$$\sigma_z^{'E'} = \begin{cases} 24.260\Delta x^{0.83660} & \Delta x < 100 \text{ m} \\ 23.331\Delta x^{0.81956} & 100 \text{ m} \le \Delta x \le 300 \text{ m} \\ 21.628\Delta x^{0.75660} & 300 \text{ m} \le \Delta x \le 1 \text{ km} \\ 21.628\Delta x^{0.63077} & 1 \text{ km} \le \Delta x \le 2 \text{ km} \\ 22.534\Delta x^{0.57154} & 2 \text{ km} \le \Delta x \le 4 \text{ km} \\ 24.703\Delta x^{0.50527} & 4 \text{ km} \le \Delta x \le 10 \text{ km} \\ 26.970\Delta x^{0.46713} & 10 \text{ km} \le \Delta x \le 20 \text{ km} \\ 35.420\Delta x^{0.37615} & 20 \text{ km} \le \Delta x \le 40 \text{ km} \\ 47.618\Delta x^{0.29592} & \Delta x > 40 \text{ km} \end{cases} \qquad \sigma_z^{'F'} = \begin{cases} 15.209\Delta x^{0.81558} & \Delta x > 200 \text{ m} \\ 14.457\Delta x^{0.78407} & 200 \text{ m} \le \Delta x \le 700 \text{ m} \\ 13.953\Delta x^{0.68465} & 700 \text{ m} \le \Delta x \le 1 \text{ km} \\ 13.953\Delta x^{0.63227} & 1 \text{ km} \le \Delta x \le 2 \text{ km} \\ 14.823\Delta x^{0.54503} & 2 \text{ km} \le \Delta x \le 3 \text{ km} \\ 16.187\Delta x^{0.46490} & 3 \text{ km} \le \Delta x \le 7 \text{ km} \\ 17.836\Delta x^{0.41500} & 7 \text{ km} \le \Delta x \le 15 \text{ km} \\ 22.651\Delta x^{0.32681} & 15 \text{ km} \le \Delta x \le 30 \text{ km} \\ 27.074\Delta x^{0.27436} & 30 \text{ km} \le \Delta x \le 60 \text{ km} \\ 34.219\Delta x^{0.21716} & \Delta x > 60 \text{ km} \end{cases} \quad (6)$$

where the σ's are in m

In (5) and (6) $0 \le \Delta x < 100$ km and PG = {'A','B','C','D','E','F'}

Notation: Δx downwind distance (m or km); PG Pasquill/Gifford stability class; σ_z^{PG} standard (Pasquill/Gifford) horizontal standard deviation (m).

Plume standard deviations derive ultimately from the spectrum of turbulence within the ambient atmosphere. Short averaging times correspond to diffusion associated with small scale eddies: long averaging times are dominated by plume meander. The distribution of vertical and horizontal turbulence differ, with the vertical turbulence materially influenced by the proximity of the ground. Turbulent kinetic energy is further influenced surface roughness: greater roughness implies greater turbulent energy, and greater eddy diffusivity.

Hanna (1982), following Smith (1973, 1977) and McDonald (1978), suggested for σ_z a surface roughness effect $(z_r/z_r^{PG})^{0.2}$. Now surface roughness governs the friction velocity u^* (say), and the Monin-Obukhov length L, with the distribution of turbulence in horizontal (σ_u/u^*, and σ_v/u^*) and vertical (σ_w/u^*) directions universal functions of the scaled height z/L (Arya 1982). Plausibly the influence of surface roughness applies equally and proportionately to the horizontal standard deviation σ_y of a dispersing plume.
However, Roberts (Chapter 5.B), analysing extensive meteorological data (Draxler 1984), discerned *no* significant effect of surface roughness upon σ_y . Certainly for longer averaging times the dominant influence upon σ_y is plume meander, which is essentially uncorrelated with

(local) surface roughness; we follow observation and take s_y independent of the surface roughness.

The influence upon horizontal standard deviation of plume meander and concentration averaging time effect has the form of the power law $(t/t_{PG})^{0.2}$ (Hanna 1982). Vertical spectra differ from horizontal as the result of the geometrical influence of the ground, so that for long averaging times no further increase in s_z with averaging time is to expected. For such times the vertical spectrum is fully active in determining turbulent diffusion. Equally for very short averaging times turbulent diffusion is dominated by small-scale eddies, the distribution of which is roughly homogeneous. This suggests that for short averaging times the functional dependence of both s_z and s_y on averaging time t should be identical, whereas, near the ground, or for long averaging times, s_z should be independent of t. We propose, following Hanna (1982) and Pasquill (1976), the dimensioned forms

Effects of surface roughness, plume centroid height, and concentration averaging-time

$$s_y = s_y^{PG} \; (t/t_{PG})^{0.2} \qquad (7)$$

$$s_z = s_z^{PG} \; (z_r/z_r^{PG})^{0.2} \; \{\min[t,t_{PG}]/t_{PG}\}^{0.2} \qquad (8)$$

with $z_r > 0$; $z_{cm} >$ ³ 0; t ³ $t_{match} > 0$

Notation: z_{cm} plume-section centroid (centre-of-mass) height (m); t concentration averaging time (s); t_{match} = 18.75 s, effectively 'instantaneous' averaging time (TNO 1990); $z_r > 0$, ground surface roughness; τ_{PG} reference averaging time (taken to be 600 s in PGPLUME); z_r^{PG} reference surface roughness height (taken to be 0.03 m (3 cm) in PGPLUME).

6.3. Local versus Integral Average Properties: Near/Far field Matching

The near-field models AEROPLUME and HFPLUME are idealised particularly in respect of the shape of the cross-wind profiles of concentration and temperature. Predictions are made not of *point-local* but of *average* behaviour within each plume cross-section, and take properly into account the several effects of source momentum, orientation, and dense gas dispersion in determining air entrainment and the development of the plume trajectory.

Far-field dispersion is similarly idealised. Predictions are made of local (particularly ground-level) concentrations; no account is taken of near source effects influencing plume trajectory. The far-field dispersion of plumes is independent of release conditions except inasmuch as they determine the downwind displacement, height above ground, and strength of an equivalent point source.

Consider an asymptotically neutral or marginally buoyant release downwind of release. In the near-field predictions are available of entrained air mass-flux, released pollutant mass-flux, and the excess (above ambient) fluxes of momentum and total energy. Sufficiently far from the source the conditions for passive dispersion of an inert pollutant are well met: chemical reaction (if pollutant is HF) has all but ceased ; the influences of release buoyancy and initial momentum largely spent.

At such distances the sectional-average predictions supplied by HFPLUME or AEROPLUME correspond closely to those of a matched Pasquill/Gifford (Gaussian) plume. Equating fluxes deduced from Gaussian far-field and 'top-hat' near-field models will then furnish a set of non-linear integral equations for the virtual source location, and will define the Pasquill/Gifford plume at the transitional or 'matching' plane and at greater distances downwind of release.

Matching Equations

$$< dm / dt >_0 = \int_0^{\infty} \int_{-\infty}^{\infty} c\, u \;\; dydz \tag{9}$$

$$< dm / dt >_{air} = \int_0^{\infty} \int_{-\infty}^{\infty} \left((\rho - c) u - \rho_\infty u_\infty \right) dydz \tag{10}$$

$$< dP_x / dt > = \int_0^{\infty} \int_{-\infty}^{\infty} \rho u (u - u_\infty) \;\; dydz \tag{11}$$

$$< dE / dt > = \int_0^{\infty} \int_{-\infty}^{\infty} \rho u \left(h + \tfrac{1}{2} u^2 - h_\infty - \tfrac{1}{2} u_\infty^2 \right) \;\; dydz \tag{12}$$

Notation: $<dm/dt>_0$ mass-flux of pollutant; $<dm/dt>_{air}$ mass-flux of entrained air, $<dP_x/dt>$ mass-flux excess (horizontal) momentum; $<dE/dt>$ mass-flux excess above ambient total-energy; (c,ρ,h,u) point-local mass-concentration pollutant, total density, specific enthalpy, and (horizontal) velocity; $(\rho_{¥},h_{¥},u_{¥})$ ambient air density, ambient air specific enthalpy, and wind speed.

The notation '<...>' refers to a *sectional-average value* such as is predicted by the HGSYSTEM near-field models AEROPLUME and HFPLUME.

The equation express the invariance between plume descriptions of $<dm/dt>_0$, the pollutant mass-flux, $<dm/dt>_{air}$, the entrained air mass-flux, $<dP_x/dt>$, the excess horizontal momentum, and $<dE/dt>$, the excess above ambient of total energy.

The pressure $P_{¥}$ within the plume is essentially that (hydrostatic) value within the undisturbed atmosphere.

Pasquill/Gifford Profiles

The assumption of a Gaussian plume/'image'-plume description of the far-field dispersion yields for the mass-concentration, and for the excess velocity the explicit profiles:

$$c/c_* = y(y,z;s_y,s_z,z_{PG})$$

$$(u - u_{¥})/(u_* - u_{¥}) = y(y,z;\varepsilon s_y,e s_z,z_{PG}) \qquad (13)$$

$$y(y,z;s_y,s_z,z_{PG}) = \exp(-y^2/(2s_y^{\,2}))\ [\exp(z - z_{PG})^2/(2s_z^{\,2})) + \exp(-(z + z_{PG})^2/(2s_z^{\,2}))]$$

with $s_y,s_z = (s_y,s_z)(Dx = x_{PG} - <x>,y = 0,z_{PG};t = t_{match},z_{cm} = <z>,z_r)$
and 0 £ z, x ³ 0, $-$¥ $< y <$ ¥ and $<z>$, s_y,s_z ³ 0.

Notation: e^2 turbulent Schmidt number; $u_* - u_{¥}$ 'centre-line' excess of horizontal velocity; $<z>$ near-field centroid height; t_{match} 'instantaneous' (concentration) averaging-time; z_r ground surface roughness.

The averaging time appropriate to the standard deviations s_y and s_z must be chosen for comparability with the near-field description underlying the entrainment assumptions of HFPLUME and AEROPLUME.
Such an averaging time is certainly short, and may be regarded as effectively 'instantaneous'. Reference to TNO(1990) yields for and 'instantaneous' average the effective averaging time $t_{match} = 18.75$ s.
Note that in addition to the expected profile for the mass concentration c(x,y,z), a second related profile has been introduced for the excess-velocity ($u(x,y,z) - u_{¥}(x,y,z)$). This reflects the broad comparability of density and velocity differences in the near-field, and the desire to assign both influences equal weight in the criteria of matching.
The velocity profile is identical in form to the Gaussian image system proposed for concentration; the standard deviations are scaled by the far-field turbulent Schmidt number ($e^2 = 1.35$) to reflect the different rates of mass and momentum diffusion (Rouse, Yih and Humphreys 1952; Ooms 1972).

Local Thermal Equilibrium

The assumption of thermal equilibrium the *point-local* thermodynamic relation

$$(h + ½u^2 - h_\infty - ½u_\infty^2) = (c/\rho)\ (<dE/dt>/<dm/dt>_0) \qquad (14)$$

to be developed.

This equation may be motivated as follows: First consider the integral-averaged plume description, and in particular the total energy-flux <dE/dt> passing a given cross-section. The mean-flow may be assumed to result from the uniform mixing of a pure pollutant stream of mass-flux $<dm/dt>_0$ with an ambient air stream of mass-flux $<dm/dt>_{air}$.

The pure pollutant stream has therefore the specific enthalpy $<dE/dt>/<dm/dt>_0$ above ambient values.

Next abstract a unit mass of pollutant/moist-air mixture from within a plume cross-section.

The sample possesses a definite mass-fraction c/ρ of pollutant: it results from the intimate mixing of two parcels of material; the one (pure pollutant) of mass c/ρ, the specific energy content of which (relative to the ambient air) is $(<c>/<p>)(<dE/dt>/<dm/dt>_0)$; the other air of mass 1 - c/ρ and *zero* specific energy (because we define the energy relative to the ambient air).

The mixture specific total energy is correspondingly $h - h_\infty + ½u^2 - ½u_\infty^2$.

The point local relationship follows from energy conservation. The non-linear equation

$$< dE / dt >= \int_0^\infty \int_{-\infty}^\infty \rho u\left(h + ½\, u^2 - h_\infty - ½\, u_\infty^2\right)\ dydz \qquad (15)$$

is then satisfied identically.

The equation system for near/far-field matching then provides a set of three non linear equations in the 'centre-line' concentration c_*, the centre-line velocity-excess $u_* - u_\infty$, and in the virtual origin location $(x_{PG}, z_{PG} \geq 0)$.

An additional equation is therefore needed to close the equation system.

Model Closure: Centroid, Buoyant Potential Energy, and Angular Momentum

Recall the importance of the plume centroid of '*centre of mass*' in model formulation: this suggests that the plume centroid height be invariable between the near and far-field descriptions. The matching equation then becomes

$$< z >= \frac{\int_0^\infty \int_{-\infty}^\infty z(\rho - \rho_\infty)\ dydz}{\int_0^\infty \int_{-\infty}^\infty (\rho - \rho_\infty)\ dydz} \qquad (16)$$

This equation is straightforward; it accurately reflects the systematic rise in the Pasquill/Gifford centroid height with increasing downwind distance, a variation not followed by the virtual source.
It differs significantly in functional form from the other matching conditions, which represent the invariance between near and far-field descriptions of the material *fluxes* whether of pollutant, entrained air, excess (horizontal) momentum, or excess total-energy.
It is suggested that the final (closure) equation should express the invariance of some physically based *flux*. Such considerations lead, rather naturally, to the invariance of the buoyancy potential-energy flux

$$< dB / dt >= \int_{0}^{\infty} \int_{-\infty}^{\infty} \rho ugz(1 - \rho_{\infty} / \rho) \, dydz \tag{17}$$

Equally some account should be taken of residual differences between plume and ambient velocities at the plane of matching; this in addition to the (hydrostatic) 'centre of gravity' effects governed by density differences alone. We suggest that the excess above ambient values of plume ***angular momentum*** be conserved.
Taking moments from the point of the matching plane of maximum ground-level concentration yields the equation

$$< dL_y / dt >= \int_{0}^{\infty} \int_{-\infty}^{\infty} \rho uz(u - u_{\infty}) \, dydz \tag{18}$$

Matching is not influenced by the choice of origin for L_y. This equation has the form of a physically derived flux, and is, in the limit of negligible velocity difference, equivalent to centroid invariance. Account is now taken of velocity differences on an equal footing with density differences analogously to the remaining conservation equations.

It is, however, *impossible* to satisfy buoyant-energy and angular-momentum flux conservation simultaneously.
This illustrates a general problem of matching, that only a *limited number* of physical invariants can be transferred between matched models, the limit being set by the Pasquill/Gifford far-field.
Introducing a velocity profile allows a rather better transfer of momentum related information than would otherwise have been possible; however it does not seem possible to introduce sufficient degrees of freedom to encompass $<dL_y/dt>$ and $<dB/dt>$ invariance.
In the circumstances we must *choose* which invariant will be conserved. Inasmuch as the buoyancy flux occurs explicitly as a major determinant of near-field behaviour, whereas the

angular momentum is only implicitly calculated, we *prefer <dB/dt> invariance* for the calculation of the far-field.

Existence of Matched (Far-field) Solutions

It is a general feature of non-linear equations that physically appropriate solutions may not exist for certain ranges of the input parameters. Certainly, circumstances may arise under which the matching of a near-field description and a far-field Pasquill/Gifford model may be inappropriate: source momentum may be significant; heavy gas effects may predominate. Even under near passive conditions sufficient 'memory' of earlier (heavy gas, say) dispersion may be retained to prevent physically sensible matching: the solution space, in terms of the matching variables $<dm/dt>_0$, $<dm/dt>_{air}$, $<dP_x/dt>$, $<dB/dt>$ needs to be examined.

This discussion is deferred until an appropriate asymptotic analysis of the non-linear system has been carried out.

6.4. System Asymptotics: the Limit of Great Dilution

Inasmuch as the Pasquill/Gifford formulation applies to *passive* dispersion, significant departures between plume and ambient atmosphere at the plane of transition are inappropriate. It is not necessary to solve the matching equations in full generality; it suffices to examine the solution space in the limit of great plume dilution.

First order expansion about the ambient state $(\rho_¥,T_¥;P_¥)$ yields estimates of the enthalpy and temperature excess above ambient, together with estimates of the centre-line concentration and velocity-excess. Vertical variation within the plume is neglected, with the wind-speed and ambient density assigned (mean) values $<u_¥>$ and $<\rho_¥>$ evaluated at the (near-field) centroid height $<z>$.

First Order Approximation

$$(h - h_¥)/(c_p^{\infty}\, T_¥) = (T/T_¥ - 1) \tag{19}$$

$$1 - T/T_¥ = (\rho/\rho_¥ - 1) + (m_¥/m_{pol} - 1)\, c/\rho_¥ \tag{20}$$

$$c_*/\rho_¥ = (b/(2p))\, (<c>/\rho_¥) \text{ with } b = <A>/(s_y s_z) \tag{21}$$

$$u_*/u_¥ - 1 = (be^2/(2p))\, (<u>/u_¥ - 1) \text{ with } b = <A>/(s_y s_z) \tag{22}$$

$$<z> = s_z Ö2\{(1/Öp)\exp(-\eta^2) + \eta\,\mathrm{erf}(\eta)\}; \text{ with } \eta = z_{PG}/(s_z Ö2) \tag{23}$$

with $½<\rho>/\rho_¥ - 1½ << 1$, $½<c>/\rho_¥½ << 1$, $½<u>/u_¥ - 1½ << 1$, $½u_¥^2/(2c_p^{\infty}\, T_¥)½ << 1$

Notation: $\mathrm{erf}(\eta) = \left(2/\sqrt{\pi}\right)\int_0^{\eta} \exp\left(-\xi^2\right) d\xi$ the standard error function (Abramowitz and Stegun 1972); c_p^{∞} ambient (moist) air (isobaric) specific heat; $m_¥$ ambient air molecular mass; m_{pol} molecular mass pollutant; (<z>,<A>) near-field plume centroid height and cross-sectional area; (<c>,<ρ>) near-field (internal-average) pollutant mass-concentration and total-density; <u> near-field (mean) flow-velocity; ($u_¥$,$\rho_¥$,$T_¥$) mean wind-speed, atmosphere density and (absolute) temperature; (ρ,c,h,T) point-local density, concentration, specific enthalpy and absolute temperature; $h_¥$ atmosphere specific enthalpy.

Note that the virtual origin is *not* located by first order matching; the quantity <A>/($s_y s_z$) being undetermined. Second order asymptotic analysis yields the required equation:

Second Order Closure

$$<A>/(s_y s_z) = 4p[D^2h + 2h_\rho d_u(d_\rho+d_u)]/[I(1,1)D^2h + 2h_\rho d_u(I(1,e)d_u + I(e,e)d_\rho)] \qquad (24)$$

where $D^2h = h_{\rho\rho}d_\rho^{\,2} + 2h_{\rho c}d_\rho d_c + h_{cc}d_c^{\,2} + 2h_\rho d_\rho^{\,2} + 2h_c d_\rho d_c$

$$I(e,\mu) = 2e^2\mu^2/(e^2 + \mu^2)\ \{1 + \exp[-2e^2\mu^2/(e^2 + \mu^2)\ (z_{PG}/\sigma_z)^2]\}$$

$$h_\rho = \rho_¥/(c_p^{\infty}\ T_¥)\ ¶(h - h_¥)/¶\rho½_{\rho\ =\ c}$$

$$h_c = \rho_¥/(c_p^{\infty}\ T_¥)\ ¶(h - h_¥)/¶c½_{c\ =\ \rho}$$

$$h_{\rho\rho} = \rho_¥^{\,2}/(c_p^{\infty}\ T_¥)\ ¶^2(h - h_¥)¶\rho^2½_{\rho\ =\ c}$$

$$h_{cc} = \rho_¥^{\,2}/(c_p^{\infty}\ T_¥)\ ¶^2(h - h_¥)¶c^2½_{c\ =\ \rho}$$

$$h_{\rho c} = \rho_¥^{\,2}/(c_p^{\infty}\ T_¥)\ ¶^2(h - h_¥)/¶\rho¶c$$

$$d_p = <\rho>/\rho_¥ - 1;\ d_c = <c>/\rho_¥;\ d_u = <u>/u_¥ - 1$$

together with the consistency constraints

$$½<u>/u_¥ - 1½½4p - be^2I(1,e)½ << 4p,\ b = <A>/(s_y s_z)$$

$$½\{(<u>/u_¥ - 1)\ [4p - be^2I(1,e)]\} + \{(<\rho>/\rho_¥ - 1)\ [4p - bI(e,e)]\}½ << 4p$$

The virtual origin is then located relative to the matching plane x= <x> at such height z_{PG} above ground, and such horizontal displacement Dx = x_{PG} - <x> that the (leading order) area and centroid matching satisfies the equation set:

Virtual Origin Location

$$<z> = s_z Ö2\{(1/Öp)\ exp(-\eta^2) + \eta erf(\eta)\} \text{ with } \eta = z_{PG}/((\sqrt{2}\cdot s_z) \qquad (25)$$

$$<A>/(s_y s_z) = 4p[D^2h + 2h_\rho d_u(d_\rho+d_u)]/[I(1,1)D^2h + 2h_\rho d_u(I(1,e)d_u + I(e,e)d_\rho)]$$

with $$D^2h = h_{\rho\rho}d_\rho{}^2 + 2h_{\rho c}d_\rho d_c + h_{cc}d_c{}^2 + 2h_\rho d_\rho{}^2 + 2h_c d_\rho d_c$$

$$I(e,\mu)=2e^2\mu^2/(e^2 + \mu^2)\{1 + exp[-2e^2\mu^2/(e^2 + \mu^2)(z_{PG}/\sigma_z)^2]\}$$

$$s_y,s_z = (s_y,s_z)(Dx = x_{PG} - <x>,z_{PG};t = t_{match},z_{cm} = <z>,z_r)$$

Notation: <x> downwind distance from release of the plane of matching; <z> near-field plume centroid at matching; t_{match} 'instantaneous' matching time; e^2 turbulent Schmidt number; <u> near-field (mean horizontal) velocity.

This non-linear system, though complex, has a *unique* solution for assumed monotone increasing standard deviations s_y and s_z and for x_{PG} £ <x>, *provided* only that $<z>/s_z$ ³ Ö(2/p); otherwise *no* solution exists.
In the absence of a solution we presume a ground-level (virtual) source, and solve for the *unique* root of the second order equation in $<A>/(s_y,s_z)$, $z_{PG} = 0$.

The solution is regular in the limit of passive dispersion, and where matching is dominated by densimetric or velocity differences; second order matching then yield the results

$$<A>/(s_y,s_z) ® 4p/I(1,1) \text{ when } <u> ® u_¥$$

$$<A>/(s_y,s_z) ® 4p/I(1,e) \text{ when } <\rho> ® \rho_¥$$

$$<A>/(s_y,s_z) = 4p/I(1,1)$$

$$<\rho> = \rho_¥$$

$$<u> = u_¥$$

$<c>$ ¹ 0

Certain consistency conditions need be imposed on the quantities $<\rho>$ and $<u>$ at matching. The empirical form of s_y is severely 'pathological' for 0 < (<x> - x_{PG}) << 10 km, that is, outside the correlated range 10 m < (<x> - x_{PG}) < 10 km, say.
Aphysical solutions so arising are very unlikely to intrude upon asymptotic matching.

6.5. Prediction of (Steady) Far-field Dispersion

Having located the virtual origin, it remains only to evaluate for each downwind displacement x ³ <x> the Pasquill/Gifford standard deviations s_y and s_z associated with the required concentration averaging-time t³ t_{match}.
Note that the vertical standard deviation s_z depends implicitly upon the local centroid (centre-of-mass) height z_{cm} via the equation

$$z_{cm} = s_z Ö2\{(1/Öp) \exp(-h^2) + h erf(h)\}; \text{ with } h = z_{PG}/(s_z Ö2) \qquad (26)$$

The solution for the pair (s_z,z_{cm}) is *unique*.
Note that for displacements for which z_{cm} > 100 m the dependence of s_z upon z_{cm} is ended, and explicit calculation recovers first s_z and then (if required) z_{cm}.
Armed with the 'width' parameters s_y and s_z, the *local concentration* at downwind distance x > <x>, height z ³0, and (horizontal) off-axis distance y is to leading order

$$c(x,y,z)/c_* = y(y,z;s_y,s_z,z_{PG}) \text{ with } c_* = dm/dt_0/[2\ p\ u_¥\ s_y\ s_z] \qquad (27)$$

where $y(y,z;s_y,s_z,z_{PG}) = \exp(-y^2/(2s_y^2))\ [\exp(-(z - z_{PG})^2/(2s_z^2)) + \exp(-(z + z_{PG})^2/(2s_z^2))]$

and 0 £ z; x_{PG} < (<x>) £ x; -¥ < y <¥; z_{PG}, s_y, s_z ³ 0

The local velocity excess is calculated similarly.

6.6. Transient Effects: Releases of Limited Duration

Thus far we have presumed that steady state conditions either exist or will develop throughout the asymptotic far-field. In practice, however, spill duration may be a few minutes; whereas the establishment of steady conditions at kilometre distances requires tens of minutes or even hours. Such different time scales are especially significant for high consequence, low probability events, for example catastrophic storage vessel failure: steady-state predictions are in such cases not merely conservative, but impossibly large. There is, therefore, a practical need for 'best estimate' values reflecting (more or less accurately) the influence of release duration upon peak concentrations in the far-field.

Downwind Diffusion

Limited duration 'puff', releases disperse both perpendicular and parallel to the ambient wind: dispersion occurs in response not only to eddy diffusion, but also (Hanna 1982) to the cumulative effect of wind-shear. We follow Ermak (1986, 1989), and Blewitt, Yohn, and Ermak (1987), in representing downwind dispersion (in the context of a Gaussian plume model) in terms of the plume standard deviation s_x. The (time/meander-averaged) standard deviation attributable to downwind diffusion is taken to be (essentially) equal to the standard deviation s_y, horizontal and perpendicular to the ambient wind. The effect of wind-shear is represented after Smith (1965), except that attention has been given to elevated as well as ground-level sources. The proposed formulation is as follows:

$$s_x^2 = s_y^2 + [2/(3p)]\, s_z^2 \, \{(du_{¥}/dz)½_{z_{cm}} \, (Dx/u_{¥})½_{z_{cm}}\}^2 \qquad (28)$$

Note that the gradient $du_{¥}/dz$ is evaluated at the plume centroid height z_{cm} rather than at Smith's (1965) reference height of $s_z/2$. This choice is representative of the (mean) wind-shear not only for grounded but also for elevated plumes. The coefficient [2/(3p)] multiplying the wind-shear term ensures predictions identical to Smith (1965) for grounded plumes and neutral stability.

Prediction of Peak Concentrations

Gaussian plume modelling is based upon the (*steady-state*) solution of the diffusion equation for a fixed point-source, uniform wind, and constant (eddy-)diffusivities. This formulation suggests the Gaussian form upon which the highly successful Pasquill/Gifford model is constructed.

Perhaps encouraged by this success, Ermak (1986) formulated a transient release model based upon the general solution of the above diffusion equation in the (Green's function) form:

$$c(x,y,z;t) = \int_{-\infty}^{\infty} (dm/dt)(\tau)\, G(x,y,z;t-\tau)\; d\tau \qquad (29)$$

with $G(x,y,z;t) = G_x(x;t)\, G_y(y)\, G_z(z)$

$$G_x(x;t) = [Ö(2/p)/s_x]\, \exp[-(x - x_{PG} - u_{¥}t)^2/(2s_x^2)]$$

$$G_y(y) = 1/[Ö(2p)s_y]\, \exp[-y^2/(2s_y^2)]$$

$$G_z(z) = 1/[Ö(2p)s_z]\ \{\exp[-(z - z_{PG})^2/(2s_z^{\,2})] + \exp[-(z + z_{PG})^2/(2s_z^{\,2})]\}$$

and $s_x(t) = Ö(2K_xt)$; $s_y(t) = Ö(2K_yt)$; $s_z(t) = Ö(2K_zt)$

Notation: dm/dt (momentary) mass release-rate (kg/s); $(x_{PG},0,y_{PG})$ location of the fixed (point) source; (K_x,K_y,K_z) eddy diffusivities parallel and perpendicular to the ambient wind; (x,y,z,t) co-ordinates and time following first release at which the (mass-) concentration c is to be evaluated.

Formally the plume standard deviations (s_x, s_y, s_z) are functions of the elapsed *time* from the moment of release. We nevertheless follow Ermak (1986) in interpreting s_x, s_y, and s_z as known (above specified) functions of the *distance* (x) downwind of a fixed source.
The (reinterpreted) solution c(x,y,z,t) forms a 'template' for a transient (Pasquill/Gifford) model or far-field diffusion. The solution c(x,y,z,t) is further simplified by presuming a *steady* source of *limited* duration. The source function dm/dt(t) assumes the form

$$\mathrm{dm}/\mathrm{dt}(t) = \begin{cases} 0 & -\infty < t < 0 \\ (\mathrm{dm}/\mathrm{dt})\big|_{\infty} & 0 < t < \tau_{\infty} \\ 0 & \tau_{\infty} < t < \infty \end{cases} \tag{30}$$

with corresponding far-field concentration

$$c(x,y,z,t)/[G_y\ G_z\ (\mathrm{dm/dt})|_{¥}] = ½\mathrm{erf}\{h/(s_xÖ2)\}\Big|_{\eta=\Delta x\text{-}u_\infty \min(0,t-\tau_\infty)}^{\eta=\Delta x-u_\infty t} \tag{31}$$

Notation: $Dx = x - x_{PG}$ distance downwind of the (virtual) point source; $\mathrm{dm/dt}|_{¥}$ (sustained) mass release-rate; $\mathrm{erf}(\eta) = \left(2/\sqrt{\pi}\right)\int_0^{\eta} \exp\left(-\xi^2\right) d\xi$ standard error function (Abramowitz and Stegun 1972).

For each downwind distance (x) the time (t) at which occurs the maximum concentration corresponds to the (unique) root of the (turning point) equation ¶c/¶t = 0.
The maximum concentration at distance x downwind of release is therefore (Ermak 1986)

$$c_{max}(x,y,z)/[G_y\,G_z\,(\mathrm{dm/dt})|_{¥}] = ½\mathrm{erf}\{(1/Ö2)\ [\min(Dx,½u_{¥}t_{¥}) + h]/s_x\}\Big|_{\eta=0}^{\eta=u_\infty\tau_\infty} \tag{32}$$

with the steady-state value recovered in the limit of infinite release duration.

Release maximum and steady-state concentrations are then related by the (dimensionless) factor

$$c_{max}/c^{steady}_{state} = \mathrm{erf}\{\surd 2\{\min(\Delta x, ½ u_{\infty} t_{\infty}) + h]/\sigma_x\}]\big|_{\eta=0}^{\eta=u_{\infty}\tau_{\infty}} / \{1 + \mathrm{erf}[\Delta x/(\sigma_x \surd 2)]\} \qquad (33)$$

which provides an *approximate* correction for the combined effects of downwind diffusion and of release duration. The correction acts upon steady-state values estimated from asymptotic matching and by the straight forward use of standard Pasquill/Gifford formulae.

6.7. Conclusions

In the far-field the calculation of plume dispersion by means of an entrainment based (integral-averaged) description is both highly uncertain and seriously inefficient. Such models as exist currently (Bloom 1980) derive entrainment from an analysis of observed dispersion behaviour summarised in the Pasquill/Gifford curves; any satisfactory formulation of entrainment must, in the far-field, recover the observed results.

Such far-field performance is best achieved by means of (asymptotic) 'matching'; that is by preserving at some matching plane a set of physically derived fluxes generated in the near-field by an integral-averaged model. This results in the identification of a virtual (point) source, such that a Pasquill/Gifford plume at the matching plane is, as regards several physical fluxes, identical to that predicted near the actual source. Beyond the matching plane, dispersion behaviour is taken to be that derived for a Pasquill/Gifford model. Approximate correction may be made for limited duration releases and for downwind diffusion using an (error function) correction suggested by Ermak (1986). The formulation, though tentative, should provide an estimate of the 'conservatism' inherent in assigning steady-state predictions to high consequence, short duration releases.

Matching is achieved in the limit of large dilution, for which buoyancy effects, mis-alignment of plume and wind, and the influence of release momentum are negligible.
Matching takes proper account of differences in vertical and horizontal diffusion, and of the influence upon these of concentration averaging times, and the proximity of the ground. Once the virtual source is located concentrations, may be predicted for *any* required averaging time, and for any point downwind of the plane of matching.

In HGSYSTEM, the far-field passive dispersion is simulated using the PGPLUME model. PGPLUME is, in effect, a 'post-processor' to AEROPLUME and HFPLUME to be used beyond the limits of AEROPLUME/HFPLUME when the near-field dispersion remains 'airborne', or at least does not credibly merge into a heavy-gas advected plume in the manner of HEGADAS (see Chapter 7.A section 7.A.4.2. for linking between the HGSYSTEM plume models and HEGADAS).

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