9. TECHNICAL DESCRIPTION OF 'MMES' OPTIONS

CONTENTS

9. TECHNICAL DESCRIPTION OF 'MMES' OPTIONS

This chapter contains a description of five special options for HGSYSTEM that were developed by The Earth Technology Corporation, USA, as part of their work on HGSYSTEM for Martin Marietta Energy Systems Inc and the U.S. Department of Energy.

These options are included in HGSYSTEM because they might be useful to some other users, and are referred to as HGSYSTEM-MMES in the following text.

The five added options are:

1. Removal by dry and wet deposition
2. Plume lift-off
3. Meteorological pre-processor
4. Concentration fluctuations and variations with averaging time
5. Effects of buildings and terrain obstacles

The full technical documentation of the work done by The Earth Technology Corporation is in the report by Hanna, Chang and Zhang (1994). This Chapter is broadly the same as Chapter 6 of the full Earth Technology report (plus relevant references).

For further information and technical support on the options described in this Chapter, the user should consult Earth Technology Corporation, 196 Baker Avenue, Concord, Massachusetts 01742-2167, U.S.A., telephone 508.371.4200, fax 508.371.4280.

9.1. Removal By Dry And Wet Deposition

9.1.1. Overview of Removal Processes

The plume will consist of a mixture of gases, solid particles, and aerosols. Larger particles and aerosols will fall to the ground due to gravitational settling. Smaller particles and aerosols and gases will deposit on the surface due to a process called dry deposition, which is caused by a combination of phenomena such as chemical reactions and physical interception by the ground and vegetation. In the presence of rain, fog, or snow, the pollutant may be removed from the plume and deposited on the ground either by absorption or collection by the water drops or snow flakes. These processes are illustrated in Figure 9-1. Thorough reviews of the topics of dry deposition and wet scavenging are given by Sehmel (1984) and Slinn (1984), respectively.

Models for hazardous gas dispersion (e.g., SLAB, DEGADIS, or HGSYSTEM) generally do not account for dry or wet deposition, since, at distances within a few hundred meters of the source, these processes are significant only for large particles (diameter D_p > 1000 μm). Most of the research on dry and wet deposition has been connected with much larger time and space scales (e.g., acid deposition over the North-eastern U.S. over time periods of several days). In addition, there has been concern about deposition of toxic substances such as dioxin which are produced at solid waste incinerators. Consequently, comprehensive wet and dry deposition modules have been built into the EPA's Regional Acid Deposition Model (RADM) and Industrial Source Complex-Version 2 (ISC-2) model.

The original research on wet and dry deposition in the 1950's was spurred by the U.S. Atomic Energy Commission's concern with fallout from nuclear weapons tests and with deposition from fuel production and reprocessing facilities (see Sehmel 1984 and Slinn 1984). The results of this work formed the basis for the models in use today.

9.1.2. Desired Complexity Level in Deposition Algorithms

Martin Marietta's PLM89A model (Bloom et al., 1989) contains some simplified dry and wet deposition formulas. These formulas have been reviewed and some formulas have been added for gravitational settling and wet removal. It is recognized that deposition is a minor component of the conservation equation for most chemicals in the plume, and it is not necessary to account for all the various details of the removal processes. Furthermore, there are large uncertainties in the required input information, such as the size spectrum for the particles formed after a flashing liquid release. Consequently, simplified default methods are suggested. If, in the future, field experiments suggest that certain details must be included, revised formulas can be developed.

The dry deposition formulas are applied as a post-processor in HGSYSTEM-MMES, given the ground level distribution of calculated concentrations. At the moment, it is assumed that there is no feedback between dry deposition and the plume chemistry and thermodynamics.

9.1.3. Removal by Gravitational Settling and Dry Deposition

Gravitational Settling of Large Particles or Aerosols

Large particles or aerosols, with diameter, D_p, greater than about 50 μm (where 1 μm = 10^{-6} m), will have a gravitational settling speed, v_s, of greater than 10 cm/s. In this case, removal is dominated by simple gravitational settling. Stoke's law can be used with a slip correction factor:

$$v_s = \frac{(\rho_p - \rho_{air}) \cdot g \cdot D_p \cdot c_2}{18 \cdot \mu} \cdot S_{CF} \qquad (9\text{-}1)$$

where,

ρ_p (g/m^3) = particle density
ρ_{air} = air density
g (9.81 m/s^2) = acceleration of gravity
D_p (μm) = particle diameter
μ = 1.81 x 10^{-4} g/cm·s = air viscosity
c_2 = 1 x 10^{-8} cm^2/μm^2 = conversion factor

and S_{CF} is the slip correction factor for larger particles:

$$S_{CF} = 1 + \frac{0.13\cdot\left(1.257 + 0.4\cdot e^{-8.5\cdot D_p}\right)}{D_p} \tag{9-2}$$

It is implied that a plume of large particles with a given diameter, D_p will fall away from the gaseous part of the plume with a speed of v_s, as illustrated in Figure 9-2. The vertical distance 'fallen' by the particle plume relative to the remainder of the gas plume at downwind distance, x, is given by $v_s x/u$. This is called the 'tilted plume' model in the literature. It is assumed that the tilted plume has the same shape as the remainder of the gas plume, but is displaced downward due to the settling of the particles.

The large particles are modelled in HGSYSTEM-MMES by the following steps:

1) Assume that the large particles can be divided into a few size classes, where each size class is characterized by a diameter, D_p, and a concentration, $C(D_p)$. The particle plume is assumed not to affect the remainder of the plume.

2) The local particle deposition flux to the ground is given by

$$F_{D_p} = v_s\, C(D_p, x, y, 0) \tag{9-3}$$

where $C(D_p,x,y,0)$ refers to the ground level concentration of that size class of particles at position (x,y) of the tilted plume.

Dry Deposition of Small Particles and Gases

Aside from the large particles, the remaining components of the plume (gas, small particles, and aerosol) do not have appreciable settling velocities. For example, in an HF plume the HF·H_2O compound is assumed by the current version of the model to be in the gas phase. But even if this compound were in the liquid phase, the HF·H_2O aerosol drops would have diameters typical of natural fogs (about 1 to 10 μm). Consequently, standard dry deposition formulas can be used to calculate the deposition to the ground surface. Also, because we are primarily interested in distances within a few hundred meters of the source, and because it is desirable in the plume thermodynamics algorithms that no mass be removed from the plume, it is assumed that the mass removal due to dry deposition is insignificant when compared to the total mass flux in the plume.

The dry deposition formula that is proposed is based on that in the EPA's revised ISC2 model, and is similar to that used in the PLM89A model by Bloom et al. (1989). Most state-of-the-art deposition models now use the resistance analogy, where the deposition velocity is assumed to be inversely proportional to the sum of a set of resistances, as expressed below:

$$v_d = \frac{1}{r_a + r_s + r_t} + v_s \tag{9-4}$$

where v_s is the gravitational settling speed, which is non-zero for particles (see equations 9-1 and 9-2) and is zero for gases.

The resistances have the following definitions:

r_a (s/m) - aerodynamic resistance
r_s (s/m) - surface or laminar layer resistance
r_t (s/m) - transfer resistance dependent on surface characteristics.

The aerodynamic resistance term is the same for both gases and small particles:

$$r_a = \frac{1}{0.4\, u_*} \left(\left(\ln\left(\frac{z_d}{z_o}\right) - \Psi_H\left(\frac{z_d}{L}\right) \right) \right) \tag{9-5}$$

where u_* is friction velocity, L is Monin-Obukhov length, z_d is reference height (assumed to equal 10 m) and the function ψ_H is given by:

$$\Psi_H\left(\frac{z}{L}\right) = -5 \cdot z / L \qquad 0 < z/L \tag{9-6a}$$

$$\Psi_H\left(\frac{z}{L}\right) = 0 \qquad z/L = 0 \tag{9-6b}$$

$$\Psi_H\left(\frac{z}{L}\right) = 2 \cdot \ln\left(\frac{1+(1-16 \cdot z/L)^{1/2}}{2}\right) \qquad z/L < 0 \qquad (9\text{-}6c)$$

The HGSYSTEM-MMES model will automatically provide values of u_* and L based on observations of wind speed and stability. The code will also provide estimates of stability class based on the surface roughness length and the estimated value of L. As a default, the following parameterizations can be made:

$$u_* = u(10\ \text{m})/15. \qquad (9\text{-}7)$$

$$L = \begin{cases} -20\ \text{m} & \text{Class A} \\ -50\ \text{m} & \text{Class B} \\ -100\ \text{m} & \text{Class C} \\ \infty & \text{Class D} \\ 50\ \text{m} & \text{Class E} \\ 20\ \text{m} & \text{Class F} \end{cases} \qquad (9\text{-}8)$$

The surface or laminar layer resistance, r_s, is dependent on the molecular diffusivity of gases or the Brownian diffusivity of particles, and can be estimated from the formula:

$$r_s = \left[Sc^n + \frac{St}{\left(1 + St^2\right)} \right]^{-1} u_*^{-1} \qquad (9\text{-}9)$$

where Sc is the Schmidt number, St is the Stokes number, and

$$n = -0.5 \text{ for } z_o < 0.1\ \text{m}$$
$$n = -0.7 \text{ for } z_o > 0.1\ \text{m} \qquad (9\text{-}10)$$

The Schmidt number is given by:

$$Sc = v / D_B \qquad \text{for particles} \qquad (9\text{-}11a)$$

$$Sc = v / D \qquad \text{for gases} \qquad (9\text{-}11b)$$

where ν is the molecular viscosity of air ($\nu = \mu/\rho = 0.15$ cm^2/s), D_B is the Brownian diffusivity of the particles in air, and D is the molecular diffusivity of the pollutant gas in air. For many gases, Sc is on the order of unity. For particles, the Brownian diffusivity, D_B, is a strong function of particle size, ranging from $D_B \sim 10^{-7}$ cm^2/s for $D_p \sim 1$ µm to $D_B \sim 0.1$ cm^2/s for $D_p \sim 10^{-4}$ µm. The ISC2 model uses the following formula to calculate Brownian diffusion D_B for particles:

$$D_B = 0.81 \cdot 10^{-9} \frac{T\, S_{CF}}{D_p} \tag{9-12}$$

where T is air temperature in K and S_{CF} is the slip correction factor (see equation 9-2). The units of D_B are cm^2/sec and the units of particle size D_p are µm.

The Stokes number is non-zero only for particles and is given by:

$$St = \left(\frac{v_s}{g}\right)\left(\frac{u_*^2}{n}\right) \tag{9-13}$$

It is evident that r_s is an important term only for gases or very small particles (diameters of 10^{-3} µm or less). r_s can be ignored for particles with sizes of about 1 µm or greater.

The third resistance term, the transfer resistance r_t, has been the subject of extensive research studies and is generally parameterized by the following formulas:

For particles,

$$r_t = r_a\, r_s\, v_s \tag{9-14a}$$

For gases,

$$r_t = \frac{1}{\frac{LAI}{r_f} + \frac{LAI}{r_{cut}} + \frac{1}{r_g}} \tag{9-14b}$$

where LAI is the leaf area index (area of leaves over a unit area of ground surface), r_f is the stomate resistance, r_{cut} is the cuticle resistance, and r_g is the resistance to transfer across the non-vegetated ground or water surface. The first two terms are significant only when vegetation is actively growing and the pollutant is sufficiently reactive to be absorbed by the vegetation. The last term is also significant only if the pollutant is reactive with the surface.

For non-reactive gases, the surface transfer resistance, r_t, is infinity and the deposition velocity is therefore zero (see equation 9-4).

The terms r_f, r_{cut}, and r_g are well-known only for gases involved in acid deposition processes, such as SO_2, NO_2, HNO_3, PAN, and O_3. For these gases, Pleim et al. (1984) suggest that r_t is on the order of 10 s/cm, with variations of ± factor of 3 depending on the particular gas.

For more highly reactive materials, set $r_t = 0.02$ s/cm in the HGSYSTEM-MMES model. If future field and laboratory studies permit r_f, r_{cut}, and r_g to be estimated, then this new information can be used to update r_t by means of equation (9-14b).

9.1.4. Removal of Particles and Gases by Precipitation and Clouds

Particles and gases can be removed from the plume by rain, snow, clouds, or fog by two mechanisms - 1) in-cloud scavenging by small cloud or fog water drops, and 2) below-cloud scavenging as large precipitation drops or snowflakes fall through a polluted plume. The first mechanism, in-cloud scavenging, is important only for reactive gases and particles, since the water drops are assumed to be not moving through the pollutant cloud, and therefore the only way the gases or particles can mix with the drops is by means of an absorption process. As Slinn (1984) explains, if the pollutant and the drops are exposed to each other for a long time, the concentration of chemicals such as SO_2 and NO_2 in the liquid reach an equilibrium determined by Henry's law. This process is clearly different from mechanism 2) above, where the liquid drops fall through the pollutant cloud in a relatively short time (a few seconds, at most) and the primary removal mechanism is via capture of pollutant particles or aerosols by the droplets.

Both in-cloud and below-cloud scavenging mechanisms can be parameterized in models using a scavenging scale, Λ, with units $(\mathrm{sec})^{-1}$, which is approximately proportional to the precipitation rate, P, with units (mm/hour). The local concentration, C, is assumed to decrease exponentially with time:

$$C(t) = C(0)\, e^{-\Lambda t} \tag{9-15}$$

where t is the time the plume has been exposed to the liquid water drops. The precipitation-induced flux of material to the ground, F_{wet}, is given by:

$$F_{wet} = \int_0^{z_w} \Lambda \cdot C(z)\, dz \tag{9-16}$$

where z_w is the depth of the wetted plume layer.

Bloom et al. (1989) include a wet removal time factor in their PLM89A model and assume that it equals 10^{-3} sec^{-1} for HF, ClF_3, and ClO_2; 2 x $10^{-3}sec^{-1}$ for UF_6 and UO_2F_2; and 0.0 for HCl, F_2 and inert substances. Ramsdell et al. (1993) use the following parameterizations for Λ for iodine gas and aerosol compounds as a function of precipitation rate in their RATCHET model:

Rain $$\Lambda = 4 \cdot 10^{-4} \; Pr^{3/4} \qquad (9\text{-}17a)$$

Snow $$\Lambda = 6 \cdot 10^{-5} \; Pr \qquad (9\text{-}17b)$$

where the precipitation rate, Pr, is in mm/hr, and the following rates are suggested.

	Pr (mm/hr liquid equivalent)		
	Light	Moderate	Heavy
Rain	0.1	3	5
Snow	0.03	1.5	3.3

For example, equation (9-17a) gives $\Lambda \approx 10^{-3}sec^{-1}$ or about $(15 \text{ minutes})^{-1}$ for moderate rain. This means that most of the pollutant would be removed after being subjected to 15 minutes of moderate rain.

It is seen that the Λ values in the PLM89A and RATCHET models are consistent. It is suggested that a default value of $(1000 \text{ sec})^{-1}$ be used in the HGSYSTEM-MMES code if the precipitation rate is not known. Equations (9-17a) and (9-17b) can be used if the precipitation rate is known. In the future, as experimental data become available, revised Λ values can be prescribed for specific chemicals such as HF-H_2O. Equation (9-16) can be used, knowing Λ and C(z), to calculate the wet flux to the ground.

Because travel times to receptors of interest would be on the order of 10 to 100 sec for accidental releases, it is possible to neglect the reduction in total mass flux due to wet deposition of chemicals in the plume. The plume chemistry and thermodynamics calculations are assumed not be affected by the wet removal at these times and distances. Of course, for larger travel times of 1000 sec or more and for distances of a few kilometers, the wet removal may be significant and may affect the plume thermodynamics.

The present version of HGSYSTEM neglects the in-cloud scavenging by fog drops, since that term is insignificant for travel times of 10 to 100 sec.

9.2. Plume Lift-Off Module

A buoyant plume blowing along the ground may 'lift off' the ground if the buoyancy forces exceed the turbulent forces within the ambient boundary layer. The few previous analyses of this problem (Briggs 1973, Meroney 1979, Poreh and Cermak 1986, Hall and Waters 1986, and Slawson et al. 1990) all dealt with plumes which tend to conserve their initial buoyancy flux, $F_o = w_o R_o^2 g(\rho_a - \rho_o)/\rho_a$, where subscript o refers to the initial plume, subscript a refers to the ambient environment, and w is plume vertical velocity, R is plume radius, g is acceleration, and ρ is density. However, a reactive plume and its subsequent products may not conserve its initial buoyancy flux, and in fact the relative plume density $(\rho_a - \rho)/\rho_a$ may change from positive to negative, depending on the influence of 1) the molecular weights of the gases that exist, 2) the enhanced effective density due to small liquid droplets and small particles carried by the plume, 3) the addition of heat due to exothermic reactions and condensation of liquids, and 4) the removal of heat due to endothermic reactions, depolymerization, and evaporation of liquids.

For example, consider a simple system where HF is released at ambient temperature and then reacts with ambient water vapor. The plume will first be very dense ($(\rho_a - \rho)/\rho_a < 0$) and may eventually be buoyant ($(\rho_a - \rho)/(\rho_a > 0$). All during this process, the plume will be growing in the vertical (depth H) and the horizontal (width W) and will be characterized by a local buoyancy flux.

$$F = (V/\pi)\, g(\rho_a - \rho)/\rho_a \qquad (9\text{-}18)$$

where V is the plume volume flux (m^3/s). For a plume of dimensions H and W which is traveling at speed u, the volume flux, V, equals uHW. Figure 9-3 shows typical time series of these variables. Also shown is the time series for the Briggs (1973) lift-off parameter, L_p, which is defined by the following expression:

$$L_p = \frac{gH(\rho_a - \rho)/\rho_a}{u_*^2} \qquad (9\text{-}19)$$

where u_* is the friction velocity (approximately given by $u_* \approx u(10\ m)/15$). The parameter L_p is proportional to the ratio of the internal plume turbulent energy due to buoyancy forces to the ambient atmospheric turbulent energy. Observations of plume lift-off in laboratory studies by the researchers mentioned above suggest that the ground-based plume will lift off the ground when $L_p \approx 20$ (there is an uncertainty of about a factor of two in this number). Prior to that point the plume may stretch vertically without lifting completely from the ground.

Note that the criterion in equation (9-19) implies that, once a plume is buoyant ($(\rho_a - \rho) > 0$), a wind speed always exists that will give $L > 20$. Assuming that $u_* = u/15$, we can use equation (9-19) to calculate that lift-off will occur when

$$u \; < \; 3.4\left(gH\left((\rho_a \; - \; \rho)/\rho_a\right)\right)^{1/2} \tag{9-20}$$

For example, if $H = 10$ m and $(\rho_a - \rho)/\rho_a = 0.01$, then lift-off will occur if $u < 3.4$ m/s. If $H = 1$ m and $(\rho_a - \rho)/\rho_a = 0.001$, then lift-off will occur only if $u < 0.34$ m/s.

Briggs and the others employ criterion (9-19) along with assumptions for the growth of volume flux, V, with time to derive formulas for calculating the distance at which $L_p = 20$ for plumes where buoyancy flux F is conserved. These formulas are not given here because F is not conserved in some reactive plumes.

The default procedure for calculating plume lift-off in HGSYSTEM is the following:

(1) Once the plume is on the ground, either because it was initially released at the ground or because it sank to the ground due to excess density, it will remain on the ground (i.e., plume base at the ground) as long as the local $L_p < 20$. Note that H and ρ are the local plume depth and density as calculated by the AEROPLUME or HEGADAS algorithms in HGSYSTEM-MMES.

(2) Once the plume depth and buoyancy increase so that the local $L_p = 20$, the plume centerline (or point of maximum concentration) is allowed to begin lifting off the ground at the rate determined by the buoyant plume vertical equation of motion in AEROPLUME or by the Briggs 'two-thirds' law' in HEGADAS.

After plume lift-off is triggered in HEGADAS, the code carries out its calculations as if the plume were still touching the ground, but the code 'remembers' that lift off is to be accounted for later. In a postprocessor, the rise of the plume centerline is calculated using the differential form of the plume rise formulas suggested by Briggs (1975) and Weil (1988):

$$\Delta z = \left(\frac{3\,\ell_b}{2\,\beta^2}\right)^{1/3} \frac{2}{3}\, x^{-1/3}\, \Delta x \tag{9-21}$$

where Δx is the integration step size, and Δz is the amount of plume rise within a downwind distance increment, Δx. The buoyancy length scale, ℓ_b, is defined by

$$\ell_b = \frac{H^2 \, g \, \Delta\rho}{u^2 \, \rho_a} \tag{9-22}$$

In the lift-off algorithm applied to HEGADAS, the height z refers to the 'bottom' of the HEGADAS plume, since that model assumes that the maximum concentration occurs at the bottom of the plume. x is the downwind distance from the point where L_p first equals 20, β is an empirical constant = 0.6, and u is the ambient wind speed (taken to be measured at 10 m). Note that ℓ_b defined in Equation (9-21) is based on the plume parameters at the point when L_p first equals 20, and is treated as a conserved quantity in subsequent calculations.

The so-called 'break-up' formula is used to determine the final buoyant plume rise. The plume will stop rising when the plume vertical velocity becomes less than the ambient turbulent velocity. The following criterion is used:

$$\frac{\frac{dz}{dt}}{1.1\, u_*} = \frac{\textit{plume vertical velocity}}{\textit{ambient}\ \sigma_w} \sim 1 \tag{9-23}$$

This criterion is satisfied when $x = \ell_b (u / u_*)^3$. It can be shown that x ~ 100 H for HEGADAS, assuming that L_p = 20 and H equals the plume depth at the point of lift-off.

9.3. Meteorological Preprocessor

9 3.1. Background

The original (NOV90 or 1.0) version of the HGSYSTEM model (McFarlane et al., 1990) had a very brief and limited meteorological processor. A few basic meteorological parameters (wind speed, stability class, surface roughness, relative humidity, temperature) are input to the model. The model uses a simple power law formula to calculate the Monin-Obukhov length, L, as a function of surface roughness and stability class, and then uses standard Monin-Obukhov similarity formulas to calculate the variation of the wind speed with height.

The cross-wind passive dispersion parameters σ_y and σ_z in the HGSYSTEM model are functions of stability class, downwind distance, surface roughness, and averaging time. The along-wind passive dispersion parameter is, in addition, a function of vertical wind shear.

The methods in the HGSYSTEM model are standard, robust procedures that have been used by modelers for over 40 years. Similar procedures are used in the PLM89A model (Bloom et al., 1989). However, as recommended by Sykes and Lewellen (1992), advanced procedures now exist for calculating boundary layer turbulence and dispersion that could be incorporated in the HGSYSTEM-MMES model. These advanced procedures can be divided into three categories of formulas:

1) Meteorological Surface Flux Formulas
2) Meteorological Profile Formulas
3) Dispersion Algorithms

Hanna et al. (1982) propose some simple formulas for each of the categories of new algorithms. For example, observations of wind speed and cloudiness could be used to estimate surface fluxes of heat and momentum. These flux estimates could then be used to generate vertical profiles of wind speed and turbulence. Finally, dispersion (σ_y and σ_z) could be calculated based on this knowledge of turbulent energy and time scales.

9 3.2. Approach to Revised Meteorological Preprocessor

State-of-the-art formulas for surface fluxes, vertical profiles, and turbulent dispersion are proposed by Hanna and Chang (1992, 1993) for their SIGPRO meteorological preprocessor and HPDM dispersion model. These are closely related to the formulas suggested by Sykes and Lewellen (1992) and to the algorithms in recent models developed by Weil (1992) and Carruthers et al. (1992).

If one were to adapt the entire set of formulas in SIGPRO and HPDM, major changes would be required to the passive dispersion algorithms in HGSYSTEM. Because the HGSYSTEM dispersion algorithms produce σ_y and σ_z estimates that are not much different from those in HPDM, it is preferable to retain the HGSYSTEM dispersion algorithms for the time being. In the future it may be appropriate to revise those passive dispersion algorithms.

As a first step, the SIGPRO and HPDM meteorological surface flux and profile preprocessors are adapted for use in HGSYSTEM. With this approach, no major revisions to HGSYSTEM are needed because that model does not currently include a major meteorological preprocessor algorithm. The codes from SIGPRO and HPDM have been directly used in the new HGSYSTEM-MMES model.

9 3.3. Description of Revised Meteorological Preprocessor

Because the two articles by Hanna and Chang (1992, 1993), describe the SIGPRO and HPDM meteorological preprocessor in great detail, the derivations are not repeated here. The reader is referred to these articles for a full discussion. For example, Section 3 of Hanna and Chang (1993) lists the assumptions and the formulas for surface heat flux Q_H, friction velocity u_*, Monin-Obukhov length L, mixing depth h, and vertical profiles of wind speed u, turbulence components (σ_v and σ_w), and temperature T.

The following input parameters are required:

z_o	surface roughness
α	surface moisture availability
L_{min}	minimum stable Monin-Obukhov length
u	wind speed at some reference height, z_{ref}
ν	solar elevation angle
N	cloud cover

The references give tables of z_o, α, and L_{min} as a function of land-use type. The reference height for the wind speed observation is usually about 10 m. The solar elevation angle (used for calculating the solar energy flux) is known from astronomical tables (e.g., the ISC2 model contains methods for determining ν from a knowledge of latitude, longitude, and time of day). The cloud cover N (ranges from 0.0 to 1.0) is observed routinely at National Weather Service stations.

To be consistent with EPA and NRC regulatory models, this revised method is designed so that it permits estimation of the Pasquill-Gifford-Turner stability class. In the new HGSYSTEM-MMES meteorological processors, the Golder (1972) nomogram (see Figure 9-4) is used, in which stability class is given as a function of z_o (in the range from 0.1 cm to 50 cm) and 1/L (in the range from -0.13 m^{-1} to 0.09 m^{-1}). The HGSYSTEM model employs this nomogram in reverse, calculating L as a function of z_o and stability class. Depending on the requirements of the regulatory agency or the project sponsors, the meteorological processor can be applied using a range of types of input parameters.

9 4. Concentration Fluctuations And Variations With Averaging Time

The effects of concentration fluctuations and averaging time are discussed in Sections 9.4.1 and 9.4.2 below for two types of receptor definitions: 1) a receptor on the plume centerline, and 2) a receptor at a fixed geometric position. Because HGSYSTEM is intended for application to the first type of receptor, the model has been modified following the suggested formulas in the first section, 9.4.1.

9.4.1. Plume Centerline Concentrations at a Given Downwind Distance

Hazardous gas models such as HGSYSTEM can predict the crosswind concentration distribution at distance x from the source for a certain averaging time, T_a. The basic model predictions of the dense gas modules are appropriate for averaging times of about two minutes, which correspond to the field data on which the dense gas algorithms are based. The predictions of the passive gas models generally refer to an averaging time of about 10 or 20 minutes, which is the averaging time for the passive gas field data used in deriving the Pasquill-Gifford-Turner σ_y and σ_z curves. Also, the HGSYSTEM prediction is for an ensemble average--that is, the average of millions of independent realizations of that particular experiment for those specific initial and boundary conditions and other input parameters. Those millions of individual realizations would themselves have a distribution about the ensemble average.

The model predictions of the ensemble average plume centerline concentration, $C_{cl}(x,T_a)$, are not keyed to any particular geographic point--the only restriction is that the downwind distance must be x. But because natural plumes meander or swing back and forth, the ensemble average centerline concentration will drop as averaging time increases, and the position of the centerline may also shift as T_a varies. The effects of averaging time on plumes are thoroughly discussed in the review report by Wilson and Simms (1985).

Consider an ensemble of concentration observations under certain initial and boundary conditions. Then the variation of the distribution of C_{cl} with T_a at a fixed x would be as shown in Figure 9-5. The box plots indicate key points on the distribution function at each T_a. The dashed line on the figure passes through the mean or median (whichever you prefer) of the distributions. If the model predictions are corrected for averaging time, T_a, the corrected ensemble average concentrations should fall along this dashed line. As averaging time, T_a, approaches 0.0 (i.e. an instantaneous snapshot of the plume), the concentration C_{cl} should approach a value representative of the instantaneous plume.

It should be mentioned that some models such as TRACE are designed to be conservative--i.e., to predict concentrations, C_{cl}, higher than the mean. The descriptions of these models do not specify the quantitative percentile (e.g. the 99th percentile) of the distribution that they are aiming for. However, if a model were designed to predict the 99th percentile at each T_a, the concentration predictions would follow the dotted line in Figure 9-5. If a model were designed to give the maximum at a given T_a for a given total sampling time (60 min, in this case) the concentration predictions would follow the dash-dot line. In this latter example, the percentile associated with the single maximum concentration would increase as T_a decreases, since the total number of concentration values equals (60 min/T_a).

Parameterizations

Most hazardous gas models that correct for averaging time are attempting to follow the dashed line in Figure 1, even though they do not articulate these conditions. In addition, most models accomplish this correction by applying a $T_a^{1/5}$ power law to the lateral dispersion coefficient, σ_y, due to ambient turbulence.

$$\frac{\sigma_y(T_{a2})}{\sigma_y(T_{a1})} = \left(\frac{T_{a2}}{T_{a1}}\right)^{1/5} \tag{9-24}$$

In order to prevent σ_y from dropping below its known value for instantaneous conditions, which would inevitably happen with equation (9-24) as $T_{a2} \to 0$, a 'minimum T_{a2}' criterion is usually applied. This is the T_{a2} which would result in σ_y equalling the following values given by Slade (1968) for instantaneous plumes or puffs:

Unstable $\sigma_{yI} = 0.14 \cdot x^{0.92}$ (9-25)
Neutral $\sigma_{yI} = 0.06 \cdot x^{0.92}$ (9-26)
Very Stable $\sigma_{yI} = 0.02 \cdot x^{0.89}$ (9-27)

For neutral conditions, this criterion is satisfied at T_{a2} equal to about 20 seconds, where it is assumed that σ_y for continuous plumes is given by the Briggs-EPA formulas. However this minimum T_{a2} is dependent on what is assumed for (1) distance x, and (2) representative averaging time for the Briggs-EPA formulas. Furthermore, equations (9-25)-(9-27) themselves are based on limited data and would have significant uncertainties (say ± 50%).

As a default parameterization, the existing formulas in HGSYSTEM for accounting for averaging time are used, with the following assumptions:

- The σ_y Briggs-EPA formulas for continuous plumes are valid for an averaging time of 10 minutes.
- The 'minimum T_a' criterion is 20 seconds.
- Equation (9-24) is valid for σ_y corrections for T_a.

The HEGADAS model above assumes that the lateral distribution in a dense gas plume is made up of a dense gas core of width W and Gaussian edges with standard deviation, σ_y. The averaging time correction is then applied only to the Gaussian edges. We depart from this approach by assuming that the averaging time correlation applies to the entire plume width:

$$\frac{C_{cl}(T_{a1})}{C_{cl}(T_{a2})} = \left(\frac{T_{a2}}{T_{a1}}\right)^{1/5} \tag{9-28}$$

If we are interested in the centerline concentration at a given averaging time at a given percentile as the distribution (see the dotted line on Figure 9-5), an assumption is needed for the form of the distribution. For in-plume fluctuations, a log-normal distribution is applicable (see Hanna, 1984):

$$P(\ln C) \ = \ \int_{-\infty}^{\ln C} p(\ln C')\ d(\ln C') \tag{9-29}$$

$$p(\ln C') \ = \ \frac{1}{\sqrt{2\pi}\ \sigma_{\ln C'}}\ e^{-\left(\ln C' \ - \ \overline{\ln C'}\right)^2/2\sigma^2_{\ln C}} \tag{9-30}$$

where P is the cumulative distribution function (ranges from 0.0 to 1.0) and p is the probability distribution function.

At small averaging times (T_a ~ 20 seconds or less), atmospheric data show that

$$\frac{\sigma_{\ln C}}{\left|\overline{\ln C}\right|} \ \approx 1.0 \tag{9-31}$$

We assume that this relation is valid and that $\sigma_{\ln C}$ decreases as averaging time increases according to the following approximation to Taylor's formula:

$$\frac{\sigma^2_{\ln C}(T_a)}{\sigma^2_{\ln C}(20 \text{ sec})} = \frac{1}{1+\dfrac{T_a}{2T_I}} \tag{9-32}$$

where T_I is the integral scale for turbulent fluctuations in concentration. For plumes in the atmospheric boundary layer, a default assumption would be

$$\text{Default} \qquad T_I \ \approx \ 300 \text{ seconds.} \tag{9-33}$$

With this value of T_I, equations (9-31) and (9-32) give

$$\sigma_{\ln C}(\text{one hour}) = 0.4 \cdot \sigma_{\ln C}(20 \text{ sec})$$

The formulas given above have been implemented in HGSYSTEM.

9.4.2. Concentrations at a given Receptor Position

The discussions in the previous subsection were concerned with predicted concentrations on the plume centerline or axis, which can shift position with time. For that type of model application, the analyst is concerned only with the maximum plume impact independent of location. The HGSYSTEM model takes that approach. Another type of model application would be concerned with the plume impact at a given receptor position, as defined by for example a monitoring site or a critical subset of the surrounding population (say a school or a hospital). The HGSYSTEM model does not currently treat this type of receptor. Nevertheless, the equations are derived below with the thought that they can be used in future modifications.

Consider an ensemble of concentration observations from a given monitoring site. The data are taken from many independent field studies, all with nearly the same ambient conditions (i.e. release rate, wind speed and direction, stability). These observations would show a variation of distribution functions with averaging time as suggested in Figure 9-6. Note that there are three major differences between Figures 9-5 and 9-6:

Figure 9-5 **Centerline C**	**Figure 9-6** **Fixed Receptor C**
Median C decreases as T_a increases	Median C is constant with T_a
There are no zeros in C	There are many zeros in C
σ_c is relatively small	σ_c is relatively large

All of these differences are due to the fact that, in the case of Figure 9-6, the plume can meander away from the receptor, leading to many C = 0 observations at that receptor. In contrast, by definition C_{cl} is always greater than zero in Figure 9-5, which is appropriate for HGSYSTEM.

Often the variation of C_{max} with T_a is calculated from data at fixed receptors. A time series C(t) is searched in order to identify the various $C_{max}(T_a)$; for example this was done by us using the field data from the Burro, Coyote, and Desert Tortoise experiments. The resulting C_{max} values would follow the dot-dashed-curve in Figure 9-6. In that example, the total length of the time series is 60 min (the sampling time T_s). The percentile of C_{max} for each T_a is given by:

$$\text{Percentile}/100 \;=\; 1 \;-\; \left(T_a / 60 \text{ min}\right) \tag{9-34}$$

Note that the variation of C_{max} with T_a is greater than the variation of C (fixed percentile) with T_a. From a theoretical point of view, C (fixed percentile) is preferable, but from a practical point of view researchers always seem to work with C_{max}. It is clearly important to at least recognize the difference.

The distribution function that is proposed for the data in Figure 9-6 must account for the possibility of many zeros. The exponential cumulative distribution function is recommended by Hanna (1984):

$$P(C) = 1 \;-\; I \exp(-IC / \overline{C}) \tag{9-35}$$

$$\sigma_c / \overline{C} = \left((2/I) - 1\right)^{1/2} \tag{9-36}$$

where I is the so-called intermittency, or fraction of non-zero observations in the total record (I = 1.0 if the plume is always impacting the receptor). A typical value of I in the atmosphere is about 0.2, giving $\sigma_c / \overline{C} = 3$. In the absence of other information, it is recommended that a default value of I = 0.2 be used for very small averaging times, T_a:

$$\left.\begin{array}{l} P(C) = 1 \;-\; 0.2 \exp(-0.2\, C / \overline{C}) \\ \sigma_c / \overline{C} = \left((2/I) \;-\; 1\right)^{1/2} = 3 \end{array}\right\} \text{as } T_a \rightarrow 0 \tag{9-37}$$

As averaging time increases to 60 minutes, equation (9-31) can be used to calculate $\sigma_c^2(T_a)/\sigma_c^2(0)$, again assuming that the integral time scale is 300 seconds and that $\sigma_c / \overline{C} = 3$ at $T_a \rightarrow 0$. 'I' can be calculated by inverting equation (9-36):

$$I \;=\; 2 / \left(1 + \left(\sigma_c / \overline{C}\right)^2\right) \tag{9-38}$$

The sequence to be followed is given below

Step 1: Calculate $$\frac{\sigma_c^2(T_a)}{\sigma_c^2(0)} = \frac{1}{1 \;+\; T_a / 600 \text{ sec}}$$

Step 2: Calculate $$I(T_a) = \frac{2}{\left(1 \;+\; \left(\sigma_c / \overline{C}\right)^2\right)}$$

Step 3: Calculate $P(C) = 1 - I \exp\left(-IC / \overline{C}\right)$

It is assumed that $\overline{C}$ is known and that $\sigma_c / \overline{C}$ $(T_a \rightarrow 0) = 3$ and hence that $I (T_a \rightarrow 0) = 0.2$.

Note: These formulas should not be used at $T_a > 3600$ sec, since the intermittency, I, would be calculated to exceed 1.0, which is impossible. Instead, use $I = 1.0$ and $\sigma_c / \overline{C} = 1.0$ at $T_a > 3600$ sec.

As mentioned above, the formulas in Section 9.4.2 for the fixed receptor position are not implemented in HGSYSTEM since the model is used to calculate concentrations for receptors on the plume centerline. Future modifications may make use of Section 9.4.2.

9.5. Effects Of Buildings And Terrain Obstacles

9.5.1. Introduction

Releases can occur in the vicinity of buildings and may be influenced by nearby terrain obstacles. These obstacles may alter the boundary layer wind flow patterns so that the trajectory and rate of dilution of the plume may be altered. In the past, hazardous gas models have ignored the influence of buildings and other obstacles because the model developers believed that these obstacles generally lead to enhanced dilution and lower concentrations.

There are several reasons why it is best to include methods for accounting for the effects of obstacles:

1. The buildings at gaseous diffusion plants, for example, are large, with relatively narrow 'canyons' between them. The plume would be constrained by the walls of the buildings.

2. Releases could occur from storage tanks and pipes within buildings, with emissions to the outside through exhaust vents on the roofs of the buildings.

3. Releases from short stacks could be mixed to the ground in the wakes of buildings, leading to increased ground level concentrations.

Simplified algorithms have been added in the HGSYSTEM-MMES code to account for these three phenomena. Later, other algorithms can be added to account for the myriad of other possible scenarios involving the effects of buildings and terrain obstacles.

9.5.2. Background

The algorithms suggested below are based on the results of a review of the effects of structures on toxic vapor dispersion carried out by Schulman, Hanna, and Britter (1990). That document drew heavily on previous reviews of the effects of structures on passive and dense gas plumes by Britter (1989) and Brighton (1989). The USAF research had the objectives of reviewing the literature on the effects of structures on toxic vapor dispersion, assessing the feasibility of producing a viable quantitative model, and determining whether the building effects were significant relative to overall model uncertainty. The literature survey followed a framework defined by a matrix based on source location and receptor location relative to the structure:

Source location?	Upwind of structure On structure Downwind of structure
Receptor location:	On face of structure In wake or cavity of structure Downwind of wake of structure

The literature was also stratified into dense gases and passive gases, and into puff and continuous plume sources. The research attempted to answer the following questions:

- Do sufficient data and mathematical models exist for developing quantitative models for the effects of structures that can be used as subroutines in existing toxic vapor dispersion models?
- Are the expected changes in concentrations due to the effects of structures significant relative to overall model uncertainties?
- Do models and data exist for trapping of toxic clouds inside large open structures?
- What is the relative accuracy of the subroutines for various source scenarios and various structure geometries?
- At what level of structure complexity do the models become inaccurate?

The results of the review suggested that sufficient information existed to develop models for a few of the source-receptor combinations listed above. In those cases, simplified formulas were suggested which are given below. In other cases, there was no information to permit even simple models to be suggested, and it would be necessary to carry out further wind tunnel or field studies to fill in the matrix. Fortunately, experimental data and empirical formulas have been developed for the three topics of interest in the current study (i.e., lateral confinement in building canyons, concentration patterns on building faces due to vent releases, and downwash into building wakes).

Most of the literature dealt with neutral or passive gases. Dense gases have not been studied as much, although it is recognized that dense gases tend to spread more laterally and less vertically.

9.5.3. Plume Confinement by Canyons

Consider the scenario shown in Figure 9-7, where the hazardous gas source is near or within a canyon between large buildings. The building height is H_B and the canyon width is W_C. Laboratory experiments by Konig (1987) and Marotske (1988) suggest that maximum concentrations are increased by a factor of as much as three due to the confinement by the canyon. This effect can be decreased if the plume height grows so that leakage occurs above the buildings.

The following simple model is proposed:

If (1) the source is between the buildings or if (2) the source is upwind of the buildings and $\sigma_y < W_C/2$ when the plume enters the canyon, and if (3) $H/H_B < 1$, then do not allow σ_y to exceed the limit:

$$\sigma_y \text{ (maximum)} = W_C / \sqrt{12} \tag{9-39}$$

This value of σ_y corresponds to a uniform lateral distribution across W_C. (Note: σ_y as used here is assumed to apply to the total plume width, not just to the plume edge.)

If $H/H_B > 1$, then only the lower part of the plume is confined by the canyon, and the upper part of the plume is free to disperse laterally as if the canyon were not there. In this case, use the following interpolation formula:

$$\text{Effective } \sigma_y \text{ (maximum)} =$$

$$\left(\frac{H_B}{H}\right)\left(\frac{W_C}{\sqrt{12}}\right)+\left(\frac{H-H_B}{H}\right)\cdot(\sigma_y\ \text{(without canyon effect)}) \qquad (9\text{-}40)$$

where σ_y (without canyon effect) refers to the lateral dispersion as ordinarily calculated by the model in the absence of obstacles. When the plume reaches the end of the canyon, lateral diffusion resumes, and a virtual source procedure should be applied to calculate concentrations further downwind.

9.5.4. Concentrations on Building Faces due to Releases from Vents

If pollutant is released accidentally within a building, it will be exhausted by vents that typically take the form of very short stacks on the roof of the building. The concentration in the plume in the exhaust vent will have been reduced by dilution through the volume of the building and most chemical reactions will have taken place (i.e., the plume will consist of small particles, gas, and aerosol). Because there will be little buoyancy to the plumes being vented, the gas can be modeled as if it were neutral or passive.

There have been many wind tunnel studies of distributions of dimensionless concentration,

$$K = \frac{CuA}{Q} \qquad (9\text{-}41)$$

on the faces of buildings of various shapes due to releases from vents on various positions on the buildings. 'A' is a representative area of the building. The source and receptors are assumed to be on the same or adjacent faces. Meroney (1982) and Wilson and Britter (1982) provide reviews of some of this work. Using the definitions in Figure 9-8, the maximum concentrations on the building at a distance, r, from the source, are given by the formulas:

$$C = 9\,Q/u_H r^2 \quad \text{for } r/A^{1/2} < 1.73 \text{ source receptor on upper } 2/3 \text{ of building} \qquad (9\text{-}42)$$

$$C = 30\,Q/u_H r^2 \quad \text{for } r/A^{1/2} < 1.73 \text{ source receptor on lower } 1/3 \text{ of building} \qquad (9\text{-}43)$$

where u_H is the wind speed at the height of the building in the flow upwind of the building, and A is the building area, assumed to equal H_B W_B.

As distance, r (the shortest distance along the surface between the source and receptor), decreases, the concentration does not increase indefinitely but should be capped by the concentration in the vent exhaust (C_{max} = Q/(volume flux from vent)).

Note that if there is a significant air flow from the vent, the vent plume may be transported up and away from the roof. In this case, the concentrations given by equations (9-42) and (9-43) would be conservative.

These formulas say nothing about the lateral or vertical extent of the plumes from the vents. Equations (9-42) and (9-43) are most useful for estimating maximum concentrations with the condition that the plume is being blown directly from the source vent to the receptor position on the building face.

The restriction that $r/A^{1/2} < 1.73$ in equations (9-42) and (9-43) is applied so that concentrations smoothly transition to the formula in the next section for the near wake (i.e., $C = 3Q/u_H A$).

9.5.5. Concentrations on the Building Downwind Face (the Near-Wake) due to Releases from Sources on the Building

This algorithm is concerned with a continuation of the vent scenario covered in the previous section. The source emissions are again assumed to be neutral or passive, and we are now concerned with the concentration in the near-wake or the recirculating cavity. This is a turbulent well-mixed zone that extends about two to five building dimensions downwind, and it is assumed that concentrations are uniform across this zone. Wilson and Britter (1982) find that the concentrations in the near wake are given by

$$C = \frac{3Q}{u_H A} \qquad \left(r / A^{1/2} \geq 1.73\right) \tag{9-44}$$

where $A = W_B H_B$ for blockish buildings and $A = H_B{}^{4/3} W_B{}^{2/3}$ for wide buildings. Figure 9-9 provides a schematic depiction of this scenario. Note that the condition $r/A^{1/2} \geq 1.73$ is applied to equation (9-44), where r is the distance from the source to the receptor.

9.5.6. Other Effects of Buildings

The three building effects covered in Sections 9.5.3, 9.5.4, and 9.6.5 are all easily handled through simple empirical formulas and all tend to increase concentration impacts. In the future, other types of effects can be included in the model as new information comes from wind tunnel and field experiments.

Some building effects have been ignored here because they tend to significantly decrease concentrations. Therefore the 'flat-terrain' solution is conservative. For example, if a source is upwind of a building, fence, or other obstacle, the increased turbulence due to the obstacle will tend to dilute the hazardous gas plume. Fences have been investigated because of their potential for mitigating the plume, and enhanced dilutions of a factor of three or more have been observed. Also, shallow dense gas plumes approaching taller obstacles are seen to be caught in the horseshoe vortices formed around the obstacle, and are therefore transported laterally away from the obstacle.

Generally, chemical reactions have been assumed to be insignificant in the simple models in the previous sections. If one were to include chemical reactions, the entrainment rate of ambient air would have to be estimated, so that the reactions of HF with water vapor could be included. Unfortunately, these entrainment rates are not well known for plumes under the influence of obstacles. Future wind tunnel studies should emphasize observations of entrainment into plumes being influenced by obstacles.

We suggest that the next algorithm that could be included in the model could be the EPA's downwash algorithm for the far wake as implemented in their Industrial Source Complex (ISC) model. This algorithm applies to the scenario when there is a stack of significant height (h_s equal to about 1 to 2 H_B) near the building and ground-level concentrations are to be calculated at a distance of about 10 H_B or greater from the stack (see Figure 9-10). The algorithm allows for enhancement of σ_y and σ_z, depending on the ratio h_s/H_B. This algorithm is not implemented in the HGSYSTEM-MMES model at the present time because (1) most sources are at the ground or at vents on the roofs of buildings, and (2) maximum impacts would occur in the near wake during the scenarios described in Sections 9.5.4 and 9.5.5.

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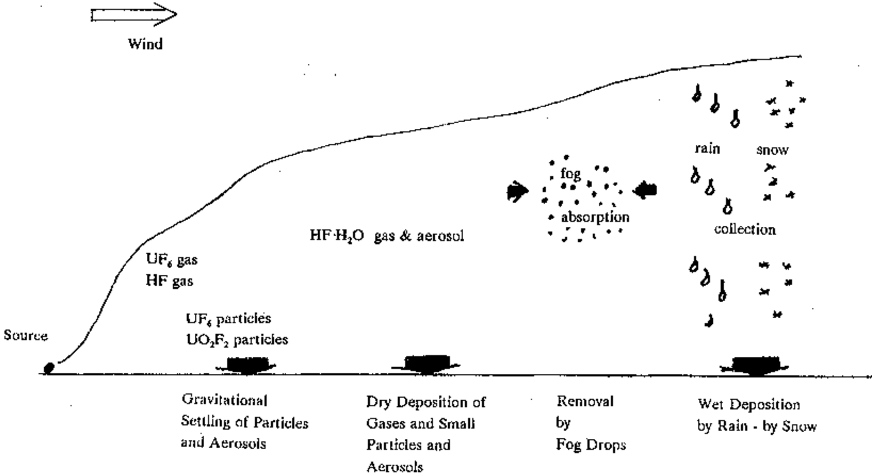


Figure 9-1. Schematic diagram of processes leading to removal of plume material by deposition to the ground.

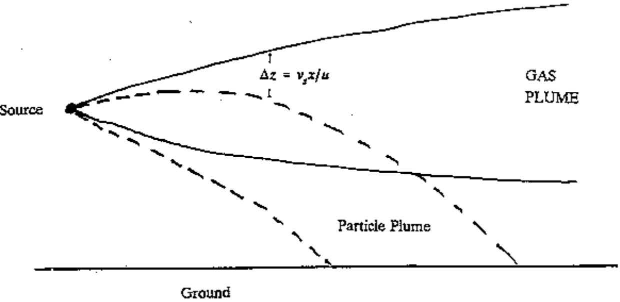


Figure 9-2. Illustration of how a large particle plume will fall away from the rest of the gas plume.

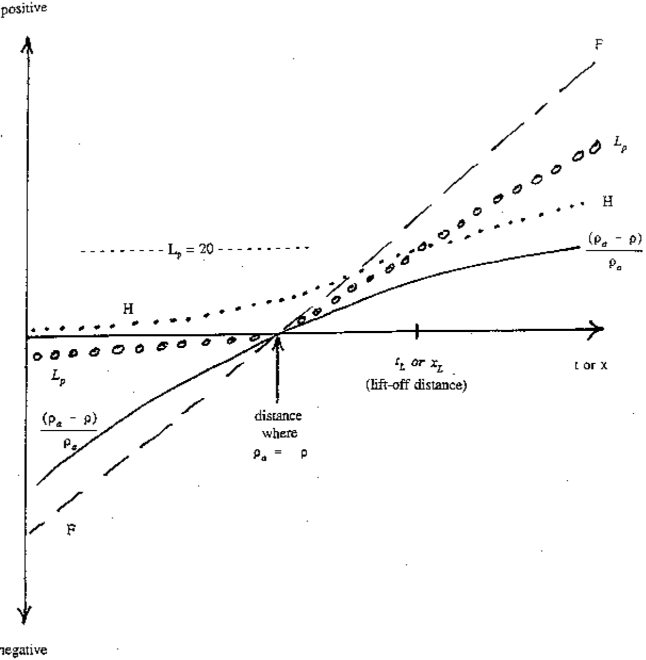


Figure 9-3. Typical time series of $(\rho_a-\rho)/\rho_a$, buoyancy force F, plume depth H, and lift-off parameter L_p for a UF_6 plume.

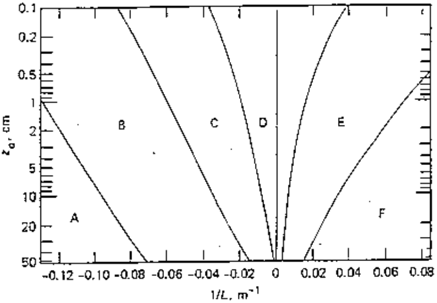


Figure 9-4. Curves showing Pasquill-Gifford-Turner turbulence types as a function of the Monin-Obukhov length and the aerodynamic roughness length. A, extremely stable conditions; B, moderately stable conditions, C, slightly unstable conditions; D, neutral conditions (applicable to heavy overcast day or night); E, slightly stable conditions; F, moderately stable conditions. [From D. Golder, Relations among stability parameters in the surface layer, *Bound. Layer Meteorol.*, **3**, 56 (1972)].

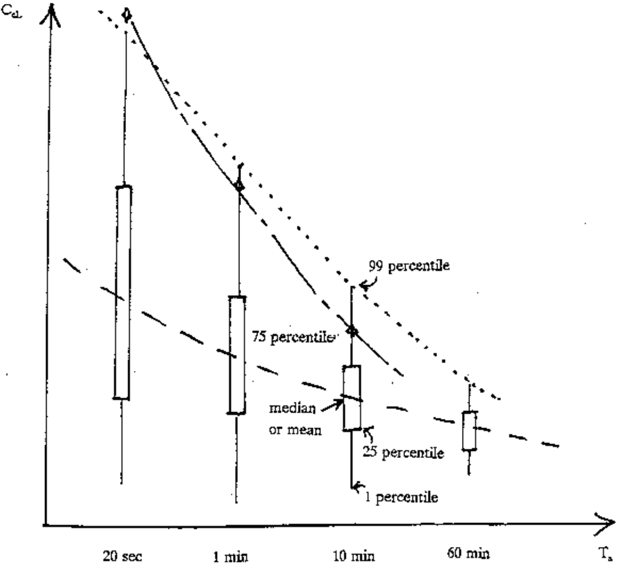


Figure 9-5. Typical distributions of centerline concentration, C_{cL}, observed at a given x, for various averaging times, T_a. The dashed line goes through the means at each T_a, and the dotted line goes through the 99th percentile of each distribution. The dashed-dotted line goes through the maximum at that T_a assuming the sampling time is 60 min.

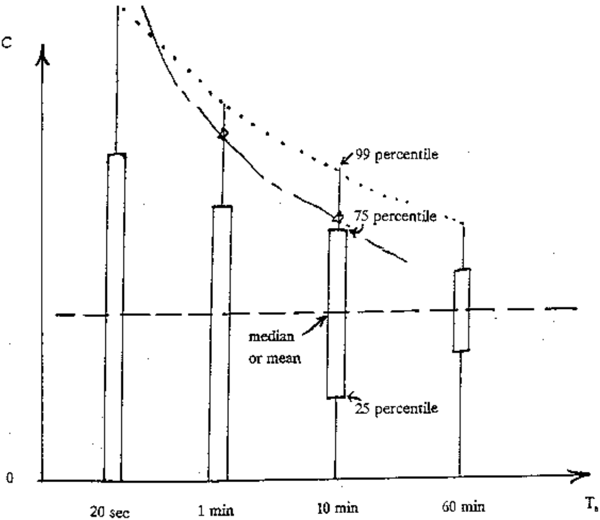
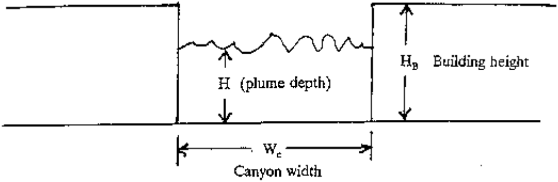
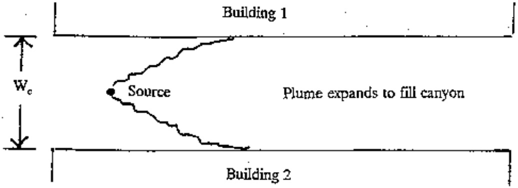


Figure 9-6. Typical distributions of concentration observed at a given monitor location, for various averaging times, T_a. The dashed line goes through the means at each T_a, and the dotted line goes through the 99th percentile of each distribution. The dashed-dotted line goes through the maximum at that T_a assuming the sampling time is 60 min.



a) Cross-section in the vertical and lateral dimensions



b) View looking down

Figure 9-7. Hazardous gas release in a canyon between buildings.

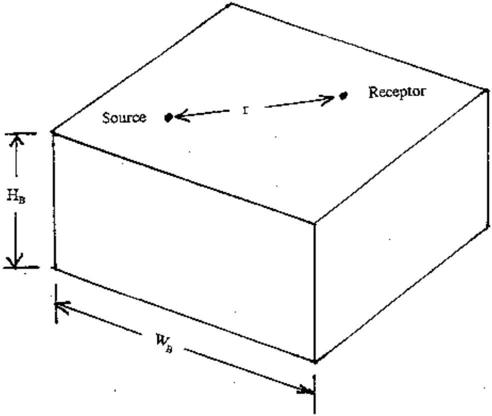


Figure 9-8. Definitions of parameters for calculating concentrations on building faces due to emissions from vents.

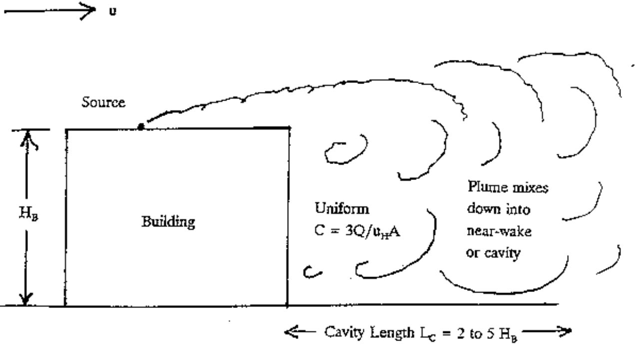


Figure 9-9. Schematic diagram of passive plume mixing into near-wake.

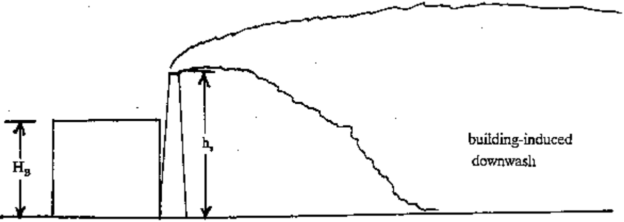


Figure 9-10. Scenario of dispersion in the far-wake, for which the ISC model downwash algorithms applicable.