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## Integrated Modeling of the Release and Dispersion of Hazardous Gases in the Atmosphere

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Accidental or uncontrolled releases of heavy, flammable, or toxic gases may occur during production, storage, or transport of such gases and may pose a serious hazard to the public. A modeling system is presented that describes the behavior of such gases during several phases: (a) release; (b) gravity spreading, heating, and air entrainment; (c) dispersion; and (d) safety assessment. Specific phenomena considered include vapor flash-off, entrainment of liquid droplets and air, evaporation from a pool, slumping, cloud heating and dilution, changing meteorological conditions, and downwind transport. The safety assessment component provides spatial distributions of time-averaged concentrations and dosages; maximum concentrations, dosages, and their locations; and isopleths for specified concentration and dosage levels. The model may be used in real-time evaluation or as a predictive tool to describe instantaneous and continuous releases from multiple sources.

Safety studies associated with toxic and flammable gases have received much attention during the last two decades. As a result of various legislation enacted recently [e.g., Toxic Substances Control Act of 1976 and Occupational Safety and Health Administration (OSHA) regulations], such studies are playing an increasingly important role in emergency planning, impact assessments, and regulatory programs. An important component of such studies is an accurate prediction of potential human exposure due to an accidental or uncontrolled release of hazardous chemicals. With this information adequate emergency measures can be formulated and put into effect to prevent and minimize the potential impacts on public safety and welfare.

The dispersion of toxic chemicals is known to be more complex than the dispersion of gases released from conventional source stacks. Some toxic gases have unique dispersion characteristics because of their negative buoyancy due to temperature or molecular weight differences with ambient air. To account for the behavior of variable-density gases, to provide flexibility in characterizing the modeling system for specific types of applications, and to facilitate continued refinement of the system, four components are used to represent the major phases:

1. Release,
2. Gravity spread,
3. Dispersion, and
4. Safety assessment.

The release phase describes the emissions released during the spill to the atmosphere. The conditions of the release may contribute to flash-off

of vapor, entrainment of liquid droplets as well as air, and the resultant formation of a cold, denser-than-air mixture.

The gravity-spread phase simulates spreading and dilution of a negatively buoyant cloud under the influence of gravity and edge mixing or entrainment. The horizontal dimension of the cloud increases due to gravity spread (slumping), and the cloud is heated from below and from air entrainment. Downwind transport is also considered during the gravity-spread phase.

The dispersion phase accounts for downwind transport and turbulent dispersion of the gas from the time at which atmospheric turbulence dominates the spread of the cloud. The safety-assessment phase output is dependent on the application and the information needs of the user. Alternative outputs may include concentrations and dosages at the grid nodes of a rectilinear grid covering the study area, maximum dosage and concentration and location, and isopleths for user-specified concentration and dosage levels.

### FORMULATION OF RELEASE PHASE

The circumstances that surround the release of gas into the atmosphere play an important part in characterizing the initial gas cloud that is formed. Significant factors include storage characteristics such as container size, pressurization, or refrigeration; release features such as release height, rupture dimensions, and escape rate; and initial gas dilution. Typical release scenarios include relief valve venting, tank or pipe leaks, and tank or pipeline failures. Events following release for each type of chemical and gas storage system vary but may be generalized as follows:

1. Buoyant gases--Gases that are buoyant on release experience buoyant plume rise, plume dilution, and subsequent Gaussian dispersion.
2. High molecular weight gases--These gases experience gravity spreading with entrainment and turbulent mixing in the atmosphere.
3. Pressurized, liquefied gases--These gases, stored as liquids at ambient temperatures and elevated pressures, exhibit gas releases from two effects: (a) flash evaporation due to a reduction of vapor pressure to reach equilibrium pressure with

the atmosphere and the concomitant reduction in temperature and (b) slow pool evaporation, which results from heat transfer to the cold liquid pool. Gravity spread and dispersion of the cold gas are also influenced by surface heating of the cloud because the vapors emitted are at the boiling temperature of the gas. As a result, cloud mixing is enhanced with heating along the cloud path.

4. Refrigerated, liquefied gases--Gases such as liquified natural gas (LNG) vapor emanate from pool evaporation after a spill. The resultant vapor is denser than air and disperses with a gravity-spread component until mixing and cloud heating cause the gas to become neutrally or positively buoyant with respect to air.

5. Refrigerated, pressurized, liquefied gases--This category combines pressurization and cooling to store gases as liquids. Accidental releases of such liquids would combine flash and pool evaporation and cloud heating.

Releases can also be subdivided based on duration and are categorized as continuous or instantaneous. Releases from storage vessels that have a duration greater than the specified simulation period are treated as continuous sources. All other sources are treated as instantaneous sources. This will require some judgment in modeling specific situations and in specifying the length of the simulation period.

#### Plume Rise of Buoyant Gases

For buoyant gases released from elevated sources, the release height ( $h_{eff}$ ) is determined from the sum of the physical source height ( $h_s$ ) and the plume rise ( $h_p$ ). The formulas developed by Briggs (1) are used to calculate the plume rise with a given set of source parameters and as a function of atmospheric stability. For unstable and neutral conditions when  $h_{eff} < H$  (i.e., plume does not rise into an elevated stable layer),

$$h_p = 1.6 F^{1/3} (3.5 x^*)^{2/3} u^{-1} \quad (1)$$

for unstable and neutral conditions when  $h_{eff} > H$  (i.e., the plume penetrates into an elevated stable layer),

$$h_p = \text{MIN} [h_{eff} (1.8 z_b^3 + 18.75 F u_m^{-1} S^{-1})^{1/3}] \quad (2)$$

for stable conditions when  $u \geq 1.37$  m/s,

$$h_p = 2.6 F^{1/3} S^{-1/3} u^{-1/3} \quad (3)$$

and for stable conditions when  $u < 1.37$  m/s,

$$h_p = 5.0 F^{1/4} S^{-3/8} \quad (4)$$

where

$$F = \text{buoyancy flux (m}^4/\text{s}^3) = (gV_f/\pi) (1 - T_s/T_a);$$

$$g = 9.8 \text{ m/s}^2;$$

$$V_f = \text{stack gas volume flow (m}^3/\text{s)};$$

$$T_s = \text{stack gas temperature (}^\circ\text{K)};$$

$$T_a = \text{ambient temperature (}^\circ\text{K)};$$

$$x^* = 34.49 F^{0.4} \text{ for } F > 55 \text{ and } 14.0 F^{0.625} \text{ for } F \leq 55;$$

$$S = \text{stability parameter} = (g/T_a) (\partial\theta/\partial z);$$

$$\partial\theta/\partial z = \text{potential temperature gradient} = 0.01^\circ\text{K/m for A, B, C, and D stability, } 0.02^\circ\text{K/m for E stability, and } 0.025^\circ\text{K/m for F stability};$$

$$h_s = \text{stack height (m)};$$

$$H = \text{mixing depth (m)};$$

$$z_b = H - h_s \text{ (m)};$$

$$u = \text{wind speed (m/s)}; \text{ and}$$

$$u_m = \text{MAX}(u, 1.37) \text{ (m/s)}.$$

If a buoyant gas is released at ground level, its release height is set equal to the actual height of the source. No adjustment in release height is made for buoyant plume rise.

#### Flash Vaporization

Pressurized liquefied gases are subject to two components of vaporization on release. In the first phase a fraction of the liquid is vaporized rapidly or flashed as the liquid vapor pressure adjusts from the pressure vessel environment to the ambient air pressure and cools the liquid to its boiling point at ambient pressure.

The fraction of released gas flashed ( $f$ ) can be determined by relating the saturated liquid enthalpy ( $h_{1s}$ ) at the storage pressure to the enthalpies of the saturated liquid and saturated vapor at ambient pressure ( $h_{1a}$  and  $h_{va}$ , respectively),

$$h_{1a} = f h_{va} + (1 - f) h_{1s} \quad (5)$$

where

$$f = \text{flash fraction,}$$

$$h_{1s} = \text{enthalpy of saturated liquid at storage pressure (cal/gm),}$$

$$h_{1a} = \text{enthalpy of saturated liquid at ambient pressure (cal/gm), and}$$

$$h_{va} = \text{enthalpy of saturated vapor at ambient pressure (cal/gm).}$$

#### Liquefied Gas Vaporization

The second phase of vaporization of liquefied gases results from heat transfer to the liquid pool from the substrate. In the typical spill for liquefied gases the liquid is spilled into an impounded area, vapor is released by flash vaporization, and heat for vaporization is added to the liquid by the substrate.

The total evaporation rate ( $\dot{M}$ ) is given by

$$\dot{M} = A L^{-1} \sum_{i=1}^n \dot{q}_i \quad (6)$$

where

$$A = \text{area of the spill (m}^2\text{),}$$

$$L = \text{latent heat of vaporization (cal/gm), and}$$

$$\dot{q}_i = \text{heat transferred to the liquid per unit area sources (n) (cal/s).}$$

The most significant heat source ( $\dot{q}_i$ ) identified is heat transfer from the substrate ( $\dot{q}_s$ ). Reid and Wang (2) express this as

$$\dot{q}_s = (k_s \rho_s c_s / \pi)^{1/2} (T_s - T_l) t^{-1/2} \quad (7)$$

where

$$k_s = \text{substrate thermal conductivity (cal/s - m - }^\circ\text{K),}$$

$$\rho_s = \text{substrate density (gm/m}^3\text{),}$$

$$c_s = \text{substrate specific heat (cal/gm),}$$

$$t = \text{time after spill (s),}$$

$$T_s = \text{substrate temperature (}^\circ\text{K), and}$$

$$T_l = \text{liquid temperature (}^\circ\text{K).}$$

This is a solution to a classical heat-conduction equation for a semiinfinite slab.

### Entrainment of Liquid Droplets and Air into Initial Cloud

If the pressure inside a storage vessel falls rapidly, the vigor of the boiling process may result in a significant fraction of the released chemical being entrained in the chemical cloud as droplets. These droplets appear to be sufficiently small such that they have negligible settling velocity. The liquid mass fraction may vary from 0.0 to 0.8 of the airborne chemical (3). In general, the liquid mass fraction increases with the release rate and the storage pressure. The position of the escape orifice also influences this fraction; an opening below liquid level may result in a large entrained liquid mass fraction even in slow leak situations.

The same values for entrained liquid mass fraction are used for instantaneous and continuous releases, which is a conservative treatment for continuous releases. The following assumed values for the fraction of nonflashed chemical that is entrained into the initial cloud provide a conservative estimate for the different storage modes:

1. Pressurized, liquefied gases--1.0 times the mass of nonflashed liquid;
2. Refrigerated, pressurized, liquefied gases--0.5 times the mass of the nonflashed liquid; and
3. Refrigerated, liquefied gases--none of the nonflashed liquid is entrained as droplets.

The vigor with which the gas escapes results in entrainment of air into the initial cloud. The quantity of air entrained depends on the nature of the release (i.e., the factors that govern the entrainment of liquid droplets). Initial dilution estimates based on actual observations result in an air-gas mass ratio of 20:1 for ammonia and freon-12 (4).

The temperature differential of the released chemical and the entrained ambient air will result in evaporation of the entrained liquid chemical droplets and the concomitant cooling of the entrained air. Deposition of entrained liquid droplets may also occur, but the assumption that all entrained liquid in the initial cloud evaporates provides a conservative estimate of the gas in the initial cloud. Another conservative assumption is that only that quantity of air needed to evaporate all liquid droplets has been entrained in the initial cloud and leaves a gas and air cloud at the boiling point of the gas. The moisture content of the air is considered in calculating the mass of entrained air, but chemical reactions between the water and released chemical are not considered.

### FORMULATION OF GRAVITY-SPREAD PHASE

The gravity-spread phase of the dispersion of dense gas encompasses the spreading and dilution of the cloud under the influence of gravity and edge mixing, as well as heating due to temperature differences among the cloud, the ground, and the entrained air. As the cloud spreads by gravity, both the heating and dilution of the cloud by the environment will vary locally and the instantaneous thermodynamic state of the cloud will show some radial and vertical gradients. However, to simplify the model formulation, the cloud is represented only by its average spatial thermodynamic state, a state that is assumed to be spatially uniform but that varies with time. That is, the model computes the evolution of the size, average temperature, density, and concentration of the cloud.

### Gravity Spread (Slumping)

Once formed, the initial cloud begins to slump as would a column of liquid (3-6). The velocity of the edge of the cloud is based on a formula for a one-dimensional density intrusion:

$$\partial R/\partial t = c\sqrt{g(\rho - \rho_a)h/\rho} \quad (8)$$

or

$$\partial R^2/\partial t = 2c\sqrt{g(\rho - \rho_a)V/\pi\rho} \quad (9)$$

where

- R = cloud radius (m),
- g = gravitational acceleration (m/s<sup>2</sup>),
- V = volume of cloud (m<sup>3</sup>),
- h = height of cloud (m),
- $\rho$  = density of cloud (gm/m<sup>3</sup>),
- $\rho_a$  = density of air (gm/m<sup>3</sup>), and
- c = 1.4 [from Germeles and Drake (6)] or 1.0 [from Van Ulden (4)].

### Entrainment of Air During Slumping Phase

During the gravity-spread phase air will be entrained both at the edges of the cloud and at the top. Entrainment at the cloud edge during this time appears to be unimportant (4). If the local velocity difference is small over the top surface of the cloud, atmospheric turbulence assumes a dominant role, and the entrainment velocity ( $U_e$ ) is dependent on a form of the Richardson number (Ri) presented by Cox and Roe (7):

$$U_e = (\alpha U_1)/Ri \text{ (m/s)} \quad (10)$$

and

$$Ri = (g\ell/U_1^2)(\rho_c - \rho_a)/\rho_a \text{ (dimensionless)} \quad (11)$$

where

- $U_1$  = longitudinal turbulence velocity (m/s),
- $\ell$  = turbulence length scale = 0.4 h where h is height of puff (m),
- $\alpha$  = entrainment constant (0.5) (dimensionless),
- $\rho_c$  = density of cloud (gm/m<sup>3</sup>), and
- $\rho_a$  = density of air (gm/m<sup>3</sup>).

The rate of air entrainment is

$$\partial m_a/\partial t = \rho_a (\pi R^2) U_e \quad (12)$$

where R is the cloud radius (m) and  $m_a$  is the mass of air (gm).

### Cloud Heating

Due to the temperature difference between the ground and the vapor, the cloud can absorb heat. An important effect is the heating of the cloud by turbulent natural convection ( $Q_c$ ), the rate at which heat is supplied per unit area. This is given by Equation 13 (8):

$$Q_c = (k_f/L) 0.1457 \{ [L^3 \rho_f^2 g \beta_f \Delta T_g / (\mu_f r)^2] [(C_p \mu / k) r] \}^{1/3} \Delta T_g \quad (13)$$

where

- $C_p$  = specific heat of mixture (cal/gm),
- $\Delta T_g$  = difference between cloud and ground temperature (°K),

f = subscript denoting quantities measured at film temperature  $(T_{\text{cloud}} + T_{\text{ground}})/2$ ,  
 L = diameter of the cloud (m),  
 $\beta$  = volumetric coefficient of expansion of cloud  $[\text{m}^3/(\text{m}^3 - ^\circ\text{K})]$ ,  
 $\mu$  = viscosity (centipoise)  $[\text{gm}/(\text{s} - \text{m})]$ , and  
 k = thermal conductivity of cloud  $[\text{cal}/(\text{s} - \text{m} - ^\circ\text{K})]$ .

or

$$Q_c = Z(\Delta T_g)^{4/3} \quad (14)$$

where Z is the coefficient of  $(\Delta T_g)^{4/3}$  in Equation 13 for the rate of cloud heating by turbulent natural convection.

The rate of temperature change then becomes (3)

$$\partial T/\partial t = [(\partial m_a/\partial t) C_{p_a} \Delta T_a + Z(\pi R^2)(\Delta T_g)^{4/3}]/(m_a C_{p_a} + m C_p) \quad (15)$$

where

$m_a$  = mass of air (gm),  
 $C_{p_a}$  = specific heat of air at constant pressure (cal/gm),  
 $\Delta T_a$  = temperature difference between the cloud and the air ( $^\circ\text{K}$ ),  
 R = radius (m),  
 $\Delta T_g$  = temperature difference between the ground and the cloud ( $^\circ\text{K}$ ),  
 m = mass of chemical in puff, and  
 $C_p$  = specific heat of chemical at constant pressure (cal/gm).

Inclusion of heating by forced convection does not alter the results significantly (9). Heating by solar radiation of heat liberated due to the dissolution of the chemical in water droplets or reaction with other chemicals has been neglected.

#### Dominance of Atmospheric Turbulence

With time the cloud of dispersing gas becomes so dilute that a conventional atmospheric model can be used. The atmospheric turbulence is taken to dominate the spread when  $\partial R/\partial t$  has decreased such that (10)

$$\partial R/\partial t = c\bar{u} \quad (16)$$

where c is a constant, depending on atmospheric stability (dimensionless), and  $\bar{u}$  is the mean wind speed (m/s).

#### FORMULATION OF ATMOSPHERIC DISPERSION PHASE

After assessing the gravitational spreading of vapors, we have estimates of the general dimensions of the spread cloud and its mean concentration. After this point, the cloud is near enough to neutral buoyancy that the usual analyses for dispersion of atmospheric pollutants may be employed.

The concentration within the cloud is described by a Gaussian puff formula (11,12). The instantaneous concentration at any point (x,y,z) for a ground-level release is given by

$$\chi(x,y,z,t) = [2Q/(2\pi)^{3/2}\sigma_y^2\sigma_z] \exp\left\{-\left[(x-Ut)^2/2\sigma_x^2\right] - \left(y^2/2\sigma_y^2\right) - \left(z^2/2\sigma_z^2\right)\right\} \quad (17)$$

where

x = distance downwind (m),  
 y = distance across the wind (m),

z = height above the ground (m),  
 U = mean wind speed (m/s),  
 t = travel time (s),  
 Q = mass of gas released (gm),  
 $\sigma_y$  = standard deviation of the puff concentration distribution in the crosswind direction (m), and  
 $\sigma_z$  = standard deviation of the puff concentration distribution in the vertical direction (m).

The puff center concentration is calculated first and then adjusted to calculate concentrations at the locations of interest. For the puff center and ground level,  $x - Ut = 0$ ,  $y = 0$ , and  $z = 0$ . Equation 17 simplifies to

$$\chi(ut,0,0;t) = 2Q/(2\pi)^{3/2}\sigma_y^2\sigma_z \quad (18)$$

where the variables are as defined for Equation 17.

A virtual point source scheme is used to account for the initial dimensions of the cloud when it makes the transition from a gravity-dominated, slumping cloud to an atmospheric turbulence-dominated, dispersing cloud. If the actual source is located a distance  $X_v$  downwind of a virtual source, then downwind travel distances are actually  $(X + X_v)$ . The value of  $X_v$  is determined to be that distance at which the center point concentration described by the Gaussian puff equation is equal to the center point concentration that occurs at the end of the gravity spread.

The Gaussian dispersion formulation used in the model includes parameters that characterize the atmospheric turbulent mixing in the vertical ( $\sigma_z$ ) and horizontal ( $\sigma_y$  and  $\sigma_x$ ) directions. Gifford (10), using the results of many experimental studies, proposed that  $\sigma_y$  and  $\sigma_z$  could be correlated with downwind distance and six atmospheric stability categories that range from A (extremely unstable) to F (moderately stable). Dispersion coefficients for both urban and rural settings are available.

#### FORMULATION OF SAFETY-ASSESSMENT PHASE

Once the downwind path and gas concentrations are calculated by the dispersion formulation, the extent of the area affected by the toxic cloud can be assessed. The hazard potential can be estimated by the spatial distribution of concentrations and dosage, maximum concentrations and dosages, as well as isopleths for specified levels of concentration and dosage.

A table may be generated that lists time after release, downwind distance of cloud center point, cloud radius, time for cloud to pass that downwind point, centerline (maximum) concentration, and dosage. The time at which the maximum concentration in the cloud is reduced to safe levels may be estimated from this table.

Line printer plots can be generated for isopleths for specified dosages and concentrations and for the spatial distribution of time-averaged concentrations at specified receptor locations. The isopleths will indicate the area that has concentrations above a specific exposure level for the predicted wind direction.

#### CONCENTRATION FLUCTUATIONS - PEAK TO MEAN RATIO

To establish some criteria for safe dispersal of toxic vapor, note that certain portions of the vapor cloud may still be locally toxic even when average concentrations are below the lower threshold limit. Thus, an additional criterion beside the mean con-

centration is needed to define the safe level. This is necessary because the concentrations predicted by the model are averaged over a specified time interval. Use of a parameter, such as the ratio of the peak concentration to the mean concentration, will help ensure that areas that have hazardous levels of gas will not likely occur when the averaged concentration is below the safe level.

Burgess and others (13) reported concentration fluctuations observed downwind of a small continuous LNG spill. They report some peak-to-average concentration fluctuations as high as 20:1. However, these tests were conducted in gusty weather and fluctuations due to meandering of the plume back and forth over the fixed sensors most likely contributed much of the variability. The American Gas Association (14) land spill tests provide some information on the large scale (tens of meters) fluctuations of interest. These data indicate peak-to-average ratios of about two or three. The American Gas Association tests were conducted under neutral or slightly gusty weather conditions.

Based on fluctuation studies from continuous and instantaneous releases at ground level (6), peak-to-average ratios of about two appear reasonable for dispersion criteria under stable weather conditions and smooth terrain (typical of conditions over water). Somewhat higher values, such as three, are more appropriate as a criterion for unstable weather. These factors can be used to estimate peak concentrations given the time-averaged concentration estimates provided by the modeling system.

#### DOSAGE CALCULATIONS

Cumulative, ground-level dosage is calculated at any specified point by using Equation 19 (15):

$$D_T(x,y,0;H) = (Q_T/\pi\sigma_y\sigma_z u) \exp[-1/2(y/\sigma_y)^2 - 1/2(H/\sigma_z)^2] \quad (19)$$

where

- $Q_T$  = total amount of gas released (gm),
- $x$  = distance downwind (m),
- $y$  = distance across the wind (m),
- $H$  = effective source height (m),
- $u$  = mean wind speed (m/s), and
- $\sigma_y, \sigma_z$  = standard deviation of the puff concentration in the cross-wind and vertical direction, respectively (m).

The units of  $D_c$  are (g-s)/m<sup>3</sup>. As a conservative estimate, the effective source height for the toxic gas cloud is taken as zero after the cloud has made the transition from the slumping phase to the dispersing phase.

#### RELEASE ALGORITHMS

As identified above, releases are categorized as instantaneous or continuous. This refers to the duration of release from the storage vessel. However, even an instantaneous source may be quasi-continuous if a pool of liquid is formed and evaporation from the pool produces a continuous release to the atmosphere. Continuous sources, whether from vessel release or pool evaporation, are simulated by superimposing a number of discrete puffs. Each puff undergoes advection in a Lagrangian sense--its time history is independent of preceding or succeeding puffs. The puff representation of continuous sources allows the model to simulate changes in meteorological parameters (e.g., wind speed and direction, atmospheric stability, and ambient temperature).

For proper simulation, the puffs must overlap

sufficiently to allow the plume to appear smooth and continuous to the sampling function. This is done by altering the advection time step. As a single puff is released at each time step, any division in the time step results in puffs being released more frequently and reduces the distance that a puff travels in one time step. The ability of the model to recreate a continuous plume is strongly influenced by the distance between adjacent puff center points. When adjacent puff center points are separated by less than a puff radius, concentrations will not vary immensely as the puff separation distance goes to zero. If the center points are separated by more than a puff width, the deviations can be large. However, since the puff dimensions after the release phase (i.e., at the site of release) are substantial, the multiple puff representation of continuous sources will be sufficiently accurate in the near field.

All sources (continuous from vessel release, continuous from pool evaporation, instantaneous from vessel release) are modeled through the same four phases of release, slumping, dispersion, and safety assessment. The release phase for puffs from vessel release is different from the release phase for puffs from pool evaporation. However, after the release phase, all puffs are treated similarly.

The release modules yield values of the total amount of gas in the puff and the dimensions of the puffs subsequent to evaporation or air entrainment, if any. The puffs undergo advection by the mean wind speed while slumping and entraining air is dictated by the gravity-spread module. When atmospheric turbulence begins to dominate the gravity spread, the virtual source scheme is used to account for the puff dimension and to convert the puff to the dispersion phase. After transition to the dispersion phase, the puffs grow in the manner described by the Gaussian puff model. The pollutant path is altered by changes in wind direction specified by the user.

If a pool of liquid is formed during the release phase, evaporation from the pool is treated in subsequent time steps. The modeling system can accommodate a pool that remains throughout the simulation or a pool that is depleted. Changes in pool area may be considered via a user-specified function.

Each puff resident on the grid is sampled, by using the puff sampling function, to evaluate the average concentration experienced at each location of interest during the previous time step. For example, consider a hypothetical puff that has the puff center point at (x,y). The puff radius is truncated at  $3\sigma_y$  during the atmospheric dispersion phase. This is a reasonable simplification because less than 1 percent of the area under a Gaussian distribution function lies beyond  $3\sigma_y$  from the peak value. During the time step considered, the points of interest within  $3\sigma_y$  of the puff center are each impacted by the hypothetical puff; each location is assigned a certain concentration increment that results from the presence of the puff during the time step  $\Delta t$ . The total concentration at the specific location is the sum of the concentration increments due to each puff impacting that location. If a continuous plume has been properly simulated, a location impacted by the plume will receive individual doses from more than one puff.

#### SUMMARY

The model system described in the paper is a highly modularized approach for simulating the release and dispersion of hazardous gases in the atmosphere. The major components cover the following four phases: (a) release; (b) gravity spread, heating, and air

entrainment; (c) dispersion; and (d) safety assessment. The modular structure facilitates refinement of the modules and also specialization for specific applications. No verification tests against field data have been completed to date, but verification tests and model comparison studies are being planned.

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## U.S. Air Force Air Weather Service Methodologies for Calculating Toxic Corridors

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Four related methods for calculating toxic corridors are described. The methods incorporate techniques that are based on the Ocean Breeze and Dry Gulch diffusion equation. Meteorological inputs include the vertical temperature difference near the ground together with the speed, direction, and variability of wind at the surface. The methods are designed for use by weather forecasters to estimate quickly the transport and dispersion of a toxic chemical accidentally released to the atmosphere. Given the source strength of the toxic chemical, the forecaster's end product is a toxic corridor for which there is a 90 percent probability that spilled or released chemicals that exceed a specified exposure limit will be contained within the dimensions of the corridor.

Air Weather Service (AWS) interest in prediction methods for quick response to emergencies involving accidental toxic chemical spills began more than 20 years ago. For background, activities beginning with the Ocean Breeze and Dry Gulch diffusion projects in 1961 represent a timely starting point. Works by Sutton (1) and Pasquill (2) provide background information on previous developments in diffusion meteorology. Not only do missile and test range safety offices need meteorological assistance to ensure that their operations can be conducted without exceeding chemical exposure limits, but forecasters must also be able to respond appropriately to the hypothetical telephone caller who says, "A truck carrying liquid chlorine has jackknifed

near the main gate, and it is spewing chlorine all over. What areas should we evacuate?" Specific meteorological systems and procedures were developed for such situations (3,4) and updated and expanded procedures have recently been published (5). These procedures allow toxic corridors based on atmospheric diffusion considerations to be calculated swiftly and provided to users such as disaster-response-force teams. These calculation procedures are simple, rapid, and suited to emergency situations. The end product is a forecast of a toxic corridor for which the probability is 90 percent that exceedances of the toxic chemical concentration, normally the short-term public emergency limit (SPEL), will be contained within the corridor.

#### TECHNICAL DEVELOPMENTS AND RESULTS

In 1962 Haugen (6) summarized the inherent difficulties in using Sutton's diffusion equation for addressing exposures to toxic chemicals that might result from TITAN II missile operations. Under similar situations concentration estimates were found to vary by up to four orders of magnitude, depending on professional judgment in the selection of input parameters for the equation. Efforts to resolve