Dispersion Model Development for Open Burn/Open Detonation Sources

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1. INTRODUCTION

The disposal of obsolete munitions, propellants, and manufacturing wastes is conducted at Department of Defense (DOD) and Department of Energy (DOE) facilities. The most common disposal method is open burning (OB) and open detonation (OD) of the material, which occurs in an earthen pit or bermed area. At present, the material destroyed in a single detonation typically ranges from 100 to 5000 lbs, whereas the quantity treated in a burn can be somewhat larger and last from minutes to an hour. OB/OD activities are restricted to daytime during unstable or near-neutral atmospheric stability.

OB/OD operations generate air pollutants and require predictions of pollutant concentrations. The pollutants include SO$_2$, NO$_x$, particulates, volatile organic compounds and toxic materials such as metals, semivolatile organics, etc. (Andrus, 1992). For large detonations ($1 - 3 \times 10^4$ lbs), natural dust entrained by the blast is an additional contaminant. Emissions from OB/OD sources have the following unique features: 1) "instantaneous" or short-duration releases of buoyant material, 2) a wide variability in the initial cloud size, shape, and height, and 3) ambient exposure times from clouds that are much less than the typical averaging times (~1 hr) of air quality standards.

Dispersion models are used to estimate pollutant concentrations given the source and meteorological conditions. However, there is currently no recommended EPA dispersion model to address OB/OD sources. The most widely-used approach is INPUFF (Petersen, 1986), a Gaussian puff model, but this has several limitations as discussed below. Due to the constraints of existing models, a model development program was initiated under the DOD/DOE Strategic Environmental Research and Development Program.

In Section 2, we give an overview of the model design which is divided into "simple" and "research" components. Sections 3 and 4 describe the simple component which includes Gaussian puff and analytic plume models. This development program is in progress and is currently limited to the unstable planetary boundary layer (PBL).

2. MODEL DESIGN CONSIDERATIONS

2.1 Background

The development of an OB/OD dispersion model has considered: 1) the limitations of existing models, 2) current knowledge of turbulence and dispersion in the PBL, and 3) a mobile meteorological platform under development.

Limitations of existing models. INPUFF has been used to model OB/OD sources and can handle dispersion from individual puffs or clouds or from a sequence of puffs in a short-duration release. Although the Gaussian puff approach is suitable for OB/OD sources, INPUFF has the following limitations: 1) It adopts dispersion parameters ($\sigma_y, \sigma_z$) from the Pasquill-Gifford (PG) curves or from Irwin's (1983) scheme. 2) It includes Briggs' (1971) plume rise expressions which apply to continuous releases rather than to instantaneous sources (puffs, clouds) and does not address thermal penetration of elevated inversions capping the PBL. 3) It assumes Gaussian velocity statistics for the turbu-
Gaussian puff model is adopted for instantaneous sources and puff, integrated-puff, and plume models for short-duration releases. For the research framework, a Lagrangian particle and/or puff approach is planned. Both frameworks will be considered for "onsite" use in a real-time operational mode using data from the mobile meteorological platform, i.e., for day-to-day decisions on OB/OD operations. The puff and plume models would be used for climatological analyses needed in risk assessments.

In modeling, the important aspects to address are: 1) all source-related features including the instantaneous or short-duration nature of the release, buoyancy-induced rise and dispersion, and cloud or plume penetration of elevated inversions, 2) relative and absolute dispersion expressions that explicitly include PBL turbulence variables, 3) meteorological variables including their vertical profiles from the mobile platform, and 4) a treatment for puff and plume dispersion about complex terrain.

The following models address points 1 and 2 above and must be expanded to include points 3 and 4. Further development also will address: 1) a more complete description of initial source effects (detonation cloud size and height) and inversion penetration, 2) a more complete PBL turbulence parameterization, 3) averaging time effects on concentration, 4) the entrained dust source term, and 5) deposition of gases and particles.

3. INSTANTANEOUS SOURCES

3.1 Dispersion Model

Concentration. For instantaneous sources or detonations, a Gaussian puff model is adopted for the short-term mean concentration \( C \) field:

\[
C = \frac{Q}{(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z} \times 
\exp \left[ - \frac{(x - Ut)^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2} - \frac{(z - h_0)^2}{2\sigma_z^2} \right],
\]

where \( Q \) is the pollutant mass released, \( U \) is the mean wind speed, \( t \) is the travel time, \( h_0 \) is the effective puff height, and \( \sigma_x, \sigma_y, \text{ and } \sigma_z \) are the puff standard deviations or relative dispersion in the \( x, y, \text{ and } z \) directions, respectively. Here, \( h_0 = h_s + \Delta h \) where \( h_s \) is the source height and \( \Delta h \) is the cloud rise due to buoyancy; \( x \) and \( y \) are the distances in the mean wind and crosswind directions.

Currently, we are considering two approaches for estimating the peak ground-level concentration (GLC) at a given \( z \): 1) the peak concentration \( C_p \) in the elevated buoyant puff, and 2) a peak found from a probability distribution of concentration at a downwind receptor. The \( C_p \) is the puff centroid...
concentration given by $C_c = Q / [(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z]$, where the relative dispersion parameters are generally different in the three directions. In the following, we assume $\sigma_x = \sigma_y = \sigma_z = \sigma$. If $C_c$ is used as an estimate of the peak concentration, an estimate must be made of the probability of it being brought to the surface; one possible method is given by Weil et al. (1995).

In the second approach, we require a functional form for the concentration probability distribution (e.g., a gamma distribution; Deardorff and Willis, 1988) and estimates of $C$ and the root-mean-square concentration fluctuation $\sigma_c$ due to an ensemble of meandering puffs. The probability distribution and the $\sigma_c$ model remain to be selected. The $C$ field including puff meandering is given by Eq. (1), but with $\sigma_x, \sigma_y, \sigma_z$ replaced by the absolute dispersion parameters—$\sigma_x, \sigma_y, \sigma_z$. A Gaussian distribution for $C$ is applicable to the SBL where the probability density function (p.d.f.) of the vertical velocity $w$ is Gaussian. However, for the CBL, a skewed $w$ p.d.f. is more consistent with laboratory and field data. A skewed p.d.f. is adopted here and is parameterized by the superposition of two Gaussian distributions (Weil, 1988).

The $C$ field due to an ensemble of meandering puffs is derived from $p_w$ following the same approach as applied to continuous plumes (Weil, 1988). The resulting expression for $C$ is

$$C = \frac{Q}{(2\pi)^{3/2} \sigma_x \sigma_y} \exp \left( -\frac{(x - Ut)^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2} \right) \times$$

$$\sum_{j=1}^{2} \frac{\lambda_j}{\sigma_{zj}} \exp \left( -\frac{(z - h_e - z_j)^2}{2\sigma_{zj}^2} \right)$$

where $\sigma_{zj} = \sigma_z j$ and $z_j = \bar{w}_j x / U$ with $j = 1, 2$. The $\lambda_j$, $\sigma_j$, and $\omega_j$ ($j = 1, 2$) are the weight, mean velocity, and standard deviation of each Gaussian p.d.f. comprising $p_w$. Equation (2) applies for short distances such that the plume interaction with the ground or elevated inversion is weak. The complete expression for $C$ includes multiple cloud reflections at the ground and PBL top.

The time-averaged concentration can be found from the dose where the partial dose is defined by $\psi(x, y, z, t) = \int_0^{t} C(x, y, z, t') dt'$. The total dose by $\psi_\infty = \psi(x, y, z, \infty)$. For clouds with short passage times over a receptor, the average concentration $C_A$ can be obtained from $C_A = \psi(t_i - \psi(t_i))/T_a$, where the averaging time $T_a = t_2 - t_1$. If the puff passage time $4\sigma_x U$ is less than $T_a$, then $C_A = \psi_\infty / T_a$.

Cloud rise and inversion penetration. Scorer (1978) combined theory and laboratory experiments to obtain the following expression for cloud rise in a neutral environment

$$\Delta h = 2.35 (M_T t + F_T t^2)^{1/4}.$$  \hspace{1cm} (3)

$M_T$ and $F_T$ are the initial momentum and buoyancy of the cloud and are given by

$$M_T = \frac{4\pi}{3} r_0 w_0 \quad \text{and} \quad F_T = \frac{g Q_T}{c p \rho_a \Theta_a},$$  \hspace{1cm} (4)

where $w_0$, $r_0$, and $Q_T$ are the initial velocity, radius, and heat content of the cloud, $g$ is the gravitational acceleration, $c_p$ is the specific heat of air, and $\rho_a$ and $\Theta_a$ are the ambient air density and potential temperature.

Scorer also found the puff radius to be $r = \alpha \Delta h$, where $\Delta h$ is the cloud top height and $\alpha$ is an empirical entrainment coefficient. $\alpha$ ranged from 0.14 to 0.5 with a mean of 0.25. The relative dispersion $\sigma_r = r / \sqrt{2}$. Using field observations, Weil (1982) confirmed that Eq. (3) was a good fit to data over a wide range of times. Thus, Eq. (3) is suitable for the initial rise of a cloud, i.e., before it is limited by stable stratification. The $Q_T$ can be determined from the mass of the detonation and its heat content, $H = 1100$ kcal/kg TNT equivalent.

For cloud penetration of an elevated density jump, results have been found from laboratory experiments in a nonturbulent environment. Richards (1961) obtained an empirical expression for the fraction $P$ of the cloud penetrating the jump: $P = 1 - 0.5 \Delta \rho_B / \Delta \rho_{T_i}$, where $\Delta \rho_B$ is the density jump and $\Delta \rho_{T_i}$ is the average density excess of the cloud when it reaches the jump. The $\Delta \rho_{T_i}$ can be estimated from $F_T$ and $r$.

The $\Delta \rho$ in a detonation cloud is related to the cloud temperature excess $\Delta \Theta$ by $\Delta \rho / \rho_a = \Delta \Theta / \Theta_a$ with $\Delta \Theta = (3/4\pi) Q_T / (\rho_a c_p r^3)$. We can then rewrite Richards' expression as $P = 1 - (2\pi/3)(\Delta \Theta / \rho_a c_p \alpha^2 h^3 / Q_T)$, where $\Delta \Theta$ is the temperature jump at $z = h$. The $h$, is assumed to be zero so that the cloud radius at the inversion is $\alpha h$. The above relationship shows the strong sensitivity of $P$ to $\alpha h$.

Figure 1 shows examples of $P$ versus the detonation mass $W$, where we have used $Q_T = W \cdot H$ and $\alpha = 0.25$. For $h = 500$ m, one can see that a significant fraction of the cloud material penetrates the temperature jump for $\Delta \Theta = 1$ or $3^\circ$C. However, for $h = 1000$ m, the $P$ is significantly reduced.

A more realistic temperature distribution above the CBL is a constant $\partial \Theta / \partial z$. Experiments simulating this distribution as well as a jump above a well-mixed layer are currently underway in a salt-stratified tank at the EFA Fluid Modeling Facility in North Carolina.
In a strong CBL, the following approximations can be made for \( z \geq 0.1h \): \( \epsilon \approx 0.4w^3/h \), \( \sigma_w \approx 0.6w \), and \( T_L \approx 0.7h/w \). (Weil, 1988). These approximations coupled with \( \epsilon = b\sigma_w^2/T_L \) lead to \( b = 0.78 \). To satisfy the long-time \( \sigma_{ra} \) limit, we must have \( a_2 = 0.62a_1 \); \( a_1 \) is estimated to be 0.57 from Thomson’s two-particle model results. The resulting parameterization for \( \sigma_{ra} \) in the CBL is

\[
\sigma_{ra} = \frac{0.36X^{3/2}}{h} \exp(-0.51X) \quad \text{with} \quad X = \frac{w_x x}{Uh}, \tag{5}
\]

where we have assumed \( t = x/U \).

To connect the short-, intermediate-, and long-time relative dispersion regimes in a continuous manner, we adopt the following parameterization:

\[
\sigma_r^2 = \sigma_{ra}^2 + \sigma_{rb}^2.
\]

For clouds dominated by buoyancy, \( \sigma_{rb} = 0.42F_T^{1/4}r^{1/2} \).

The total or absolute dispersion is necessary to estimate the \( C \) for a meandering puff or plume. The \( \sigma_x \) and \( \sigma_y \) in Eq. (2) can be obtained from a parameterization of Taylor’s theory:

\[
\sigma_x = \sigma_u t/(1 + t/2T_{Lz})^{1/2} \quad \text{and similarly for} \quad \sigma_y.
\]

The \( T_{Lz} \) is the Lagrangian time scale for the \( u \) component and can be parameterized by \( T_{Lz} = (\sigma_{rb}/u_h)^2 \), etc. (e.g., see Venkatram and Wyngaard, 1988). For the CBL and the results below, we use \( T_{Lz} = T_{Ly} = 0.7h/w_u \) and \( \sigma_u = \sigma_v = 0.6w \).

3.2 Some Results

We have computed the \( C_r \) in the buoyant puff and the mean GLC along \( y = 0 \) due to a meandering puff for \( 0.1 < W < 50 \) tons. The \( \sigma_r \), \( \sigma_x \), and \( \sigma_y \) were calculated as described above. In the following, the cloud buoyancy is characterized by its dimensionless value

\[
F_{T*} = \frac{F_T}{w_x^2 h^2}; \tag{6}
\]

we used \( w_x = 2 \) m/s, \( h = 1000 \) m, and \( U = 5 \) m/s.

Figure 2 shows the dimensionless concentration \( C_{C,h^2/Q} \) as a function of \( X \). We have neglected cloud penetration of the inversion but included cloud reflection at \( z = 0, h \) and assumed that \( h_c = \text{Min}(\Delta h, h) \). The large variation in the dimensionless \( C_c \) at short range \( (X < 1) \) is due to the buoyancy-induced dispersion \( \sigma_{ra} \). As can be seen, \( C_c h^2/Q \) decreases systematically and significantly with an increase in \( F_{T*} \) due to the increase in \( \sigma_{rb} \) with \( F_{T*} \). For \( X > 1 \), the curves converge to the same limit because at long times the \( \sigma_r \) is dominated by \( \sigma_{ra} \), which is independent of \( F_T \).
Figure 3 shows dimensional values of the peak \( C_c \) \( \text{SO}_2 \) concentrations in the cloud, with \( Q = W \cdot E_f \) where \( E_f = 2.23 \times 10^{-4} \); Andrulis, 1992) is the \( \text{SO}_2 \) emission factor. In Fig. 3, the order of the curves is reversed from Fig. 1—the curve for \( W = 50 \) tons exhibits the highest \( C_c \). The reversal is due to the increase in \( Q \) with \( W \), which overcomes the decrease in \( C_c \) due to the increase in \( \sigma_{x_0} \) with \( F_T \). At small \( x \), all of the curves have the same slope: \( C_c \propto x^{-3/2} \) because \( \sigma_{x_0} \propto x^{1/2} \). Some curves exhibit a short region of a nearly constant \( C_c \) with \( x \); this is due to puff trapping in the CBL. At large distances (\( x > 10 \) km), clouds for all cases become uniformly mixed in the vertical but continue to spread laterally; thus, \( C_c \propto Q/\sigma_{x_0}^2 \propto Q/x \) as shown.

The dimensionless mean GLC, \( C_{m}^{3}/Q \), along the puff centerline is shown in Fig. 4; this mean is for an ensemble of meandering puffs and is obtained from Eq. (2) with reflection terms included. Again, the highest dimensionless concentration occurs for the smallest \( F_T \); this is attributed to the smaller \( \Delta h \) for the smaller detonations. Likewise, the increase in the distance to the maximum concentration with \( F_T \) is due to the increase in \( \Delta h \). Note that for \( x < 1 \), the \( C_{m}^{3}/Q \) can be two orders of magnitude smaller than the \( C_n x^3/Q \) (Fig. 2) at the same \( x \) value, but at \( x \approx 10 \), the curves from both figures converge to the same limit. This occurs because the puff becomes uniformly mixed in \( z \) and the \( \sigma_{x_0}, \sigma_{y_0} \approx \sigma_{x_0} \) at large \( t \) or \( x \).

Figure 5 shows the mean dimensionless GLC for the same range of \( W \) and \( F_T \) values as in Figs. 2 - 4. Several interesting features are found: 1) A non-monotonic variation occurs in the maximum GLC \( C_{m} \) with \( W \) and \( F_T \). 2) The variation in \( C_{m} \) for \( 0.1 \leq W \leq 50 \) tons is only about a factor of 4 even though the range in \( Q \) is a factor of 500; the weak dependence on \( Q \) is attributed to the increase in \( \Delta h \) with \( F_T \). 3) The \( C_{m} \) is of the order of 0.1 \( \mu g/m^3 \), which is the lower bound for \( C_c \) in Fig. 3.

We should clarify again the meaning and use of \( C \) in Figs. 4 and 5. It is the mean GLC along \( y = 0 \) due to an ensemble of meandering puffs and probably has little to do with an observed centerline GLC in an individual puff. This computed \( C \) is to be used together with a modeled \( \sigma_{x_0} \) in a concentration probability distribution to estimate the peak short-term GLC that could occur downstream of the detonation. The peak GLC would correspond to some specified probability level.

4. SHORT-DURATION RELEASES

4.1 Dispersion Model

For short-duration releases or burns, our general approach is an integrated puff model in which the short-term mean concentration relative to the puff centerline is

\[
C = \int_{0}^{t_r} \frac{Q_r \cdot f(t') \cdot dt'}{(2\pi)^{3/2} \sigma_{rz} \sigma_{ry} \sigma_{rz}} \quad (7a)
\]

\[
f = \exp \left[ -\frac{(x-U(t-t'))^2}{2\sigma_{rz}^2} - \frac{y^2}{2\sigma_{ry}^2} - \frac{z^2}{2\sigma_{rz}^2} \right] \quad (7b)
\]

where \( t' \) is the puff emission time, \( t_r \) is the total release duration, \( Q_r \) is the continuous source emission rate, \( z' = z - h_x, \sigma_{rz} = \sigma_{rz}(t - t') \), and similarly for \( \sigma_{ry}, \sigma_{rz} \). The integration in (7a) can be carried out analytically for limiting forms of \( \sigma_{rz}(t - t') \), etc., but must be done numerically.
in general. Numerical integration is required when using the parameterization $\sigma_{xy} = \sigma_{rz} = \sigma_y = \sigma_r = a_1 \epsilon^{1/2} (t - t')^{3/2} / (1 + \alpha_3 (t - t') / T_L$.

The integrated puff model also can be used for the mean concentration of meandering puffs by replacing the relative dispersion by the absolute dispersion.

In the following, we focus on the $C_c$ for a short-duration release (burn) and consider two limiting cases. 1) For $t < t_r$, we expect the rise and dispersion of the integrated puff to reduce to that of a continuous plume for sufficiently strong winds such that the relative dispersion in the $x$ direction can be neglected. 2) For $t > t_r$, the field should reduce to that for an instantaneous puff but with $Q = Q_r t_r$ and $F_r = (4 \pi / 3) F_b t_r$, where $F_b = w_0 r_0^2 g \Delta Q / \theta$ is the continuous source buoyancy flux. As will be shown below, the $C_c$ for the long-time puff solution is lower than that for the plume solution. Thus, we take the plume solution as an upper bound and $C_c = \text{Min}(C_{cpl}, C_{cpl})$, where $C_{cpl}$ and $C_{cpp}$ denote the $C_c$ values for the plume and puff, respectively.

The mean concentration field relative to the plume centerline is given by

$$C = \frac{Q_r}{2 \pi U \sigma_{xy} \sigma_{rz}} \exp \left( - \frac{y^2}{2 \sigma_{xy}^2} - \frac{(z - h_r)^2}{2 \sigma_{rz}^2} \right). \quad (8)$$

Here, the plume rise is attributed to buoyancy and is given by $\Delta h = 1.6 F_b^{1/3} x_2^{2/3} / U$ and its radius is $r = 0.42 h$ (Briggs, 1984). Source momentum effects can be included in the future. As with the puff model, we will assume $\sigma_{xy} = \sigma_{rz} = \sigma_y = \sigma_r = a_1 \epsilon^{1/2} (t - t')^{3/2} / (1 + \alpha_3 (t - t') / T_L)$. We ignore the dependence of $\Delta h$ on $t'$. The result is

$$C = \frac{Q_r}{4 \pi \sigma_y^2} \exp \left( \frac{U}{2 \sigma_y^2 T_L} (x - r) \right) \times$$

$$\left[ \text{erf} \left( \frac{r - U (t - t_r)}{\sqrt{2 \sigma_r}} \right) - \text{erf} \left( \frac{r - U t}{\sqrt{2 \sigma_r}} \right) \right], \quad (9)$$

where er is the error function and $r^2 = x^2 + y^2 + (z - h_r)^2$. We evaluate this expression at $t$ corresponding to the center of the cloud, $x = U(t - t_r / 2)$, or $t = x / U + t_r / 2$. The $C_c$ found to be $C_c = Q_r t_r / [(2 \pi)^{1/2} \sigma_r^2]$. This result supports the use of the instantaneous puff model, with $Q = Q_r t_r$, for the long-time limit of a finite-duration release.

4.2 Some Results

Results are presented for the dimensionless concentration $C_c U h^2 / Q_c$ for the plume and instantaneous puff models, with reflection at $z = 0, h$ included in both. The continuous source buoyancy flux is characterized by its dimensionless value:

$$F_* = \frac{F_b}{U w_0 h}. \quad (10)$$

Figure 6 shows the dimensionless $C_c$ for the plume model with $F_*$ in the range 0.001 $\leq F_* \leq 0.3$. The trends appear similar to those for the puff model in Fig. 2 although the variation of $C_c U h^2 / Q_c$ with $F_*$ is not as great as for the puff model. For $X < 1$, the decrease in the dimensionless $C_c$ with increasing $F_*$ is due to the increase in $\sigma_{xy}$ with $F_b$. For $X > 1$, all of the curves approach the same asymptotic curve; this is due to the dominance of $\sigma_{xy}$ at large times and its independence of $F_b$.

Figure 7 presents the dimensionless $C_c$ for both the plume and puff models for $F_* = 0.001$ and 0.01 and various values of $t_r = t_r w_0 / h$. The time scale $h / w_0 = 500 s$ for the $w_0 (= 2 m/s)$ and $h (= 1000 m)$ used here, so that $t_r$ ranges from 50 s to 500 s or about 1 to 8 min. The plume $C_c$ is chosen as long as it exceeds the puff $C_c$. As can be seen, the distance over which the plume solution applies increases as $t_r$ does.

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Fig. 6. Dimensionless concentration at plume centroid versus dimensionless downwind distance.

Fig. 7. Dimensionless concentration at plume and puff centroid versus dimensionless downwind distance.

6. REFERENCES


