Assessing Atmospheric Releases of Hazardous Materials

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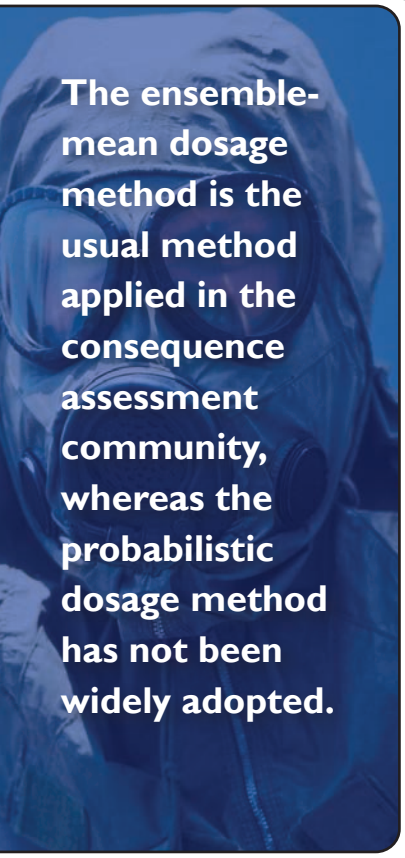
The Problem

Atmospheric transport and dispersion (AT&D) models play an important role in the Department of Defense because of the threat of battlefield or terrorist use of chemical and biological weapons. There is a need to accurately model the consequences of the intentional or accidental release of hazardous materials into the atmosphere.



The ensemble-mean dosage method is the usual method applied in the consequence assessment community, whereas the probabilistic dosage method has not been widely adopted.

Casualty estimation requires toxicological models that relate chemical exposures to toxic effects on humans. A common assumption is that toxic effects are functions of only the total inhaled dose, which in turn is proportional to the atmospheric dosage (a measure of exposure). When the dosage $D(\mathbf{x})$ at location $\mathbf{x}$ results from a steady exposure, of duration T, to a toxic agent with an atmospheric concentration $C(\mathbf{x})$ (Equation 1), these assumptions are embodied in what is called Haber's law of toxicity.

$$D(\mathbf{x}) = C(\mathbf{x})T \tag{1}$$

While Haber's Law originally was defined for constant concentrations only, the following simple extension of Haber's Law to the case of a dosage $d(\mathbf{x})$ derived from a time-varying concentration $c(\mathbf{x},t)$ (Equation 2) is quite prevalent, although it is not based on empirical data (Sommerville et al., 2006).

$$d(\mathbf{x}) = \int c(\mathbf{x},t)dt \tag{2}$$

For any given level of exposure, there is a need to estimate the associated toxic effects. The typical toxicological response model used for consequence assessments of toxic releases is a probit model based on a log-normal distribution described by two parameters: the median effective dosage Eff_{50} and the probit slope b. Equation 3 gives the probability of casualty (or fractional casualties) for a given dosage d:

$$Cas(d) = \Phi\left(b\log_{10}\left(\frac{d}{Eff_{50}}\right)\right) \tag{3}$$

where $\Phi(\bullet)$ denotes the standard normal cumulative distribution function and Eff_{50} is the dosage required to achieve a certain effect (e.g., death, incapacitation) in 50% of the population.

The majority of AT&D models used for consequence assessment predict only a "mean" plume that approximates

the ensemble average over a large number of possible turbulent plume realizations. A few AT&D models, in addition to predicting an ensemble-mean dosage or concentration, also include statistical estimates of the variance around the ensemble mean. One example is the Second Order Closure Integrated Puff (SCIPUFF) model (Sykes et al., 2007), which is incorporated in the HPAC modeling system maintained and distributed by the U.S. Defense Threat Reduction Agency (DTRA). The dosage field for a single turbulent realization of the toxic plume, $d(\mathbf{x})$, can be decomposed as

$$d(\mathbf{x}) = \overline{d(\mathbf{x})} + d'(\mathbf{x}) \qquad (4)$$

where the overbar denotes the ensemble mean and the prime denotes the turbulent fluctuation about the mean for the single realization. HPAC makes physics-based predictions of the pair $(\overline{d(\mathbf{x})}, \overline{d'^2(\mathbf{x})})$ at each prescribed location $\mathbf{x}$, where $\overline{d(\mathbf{x})}$ is the ensemble-mean dosage and $\overline{d'^2}(\mathbf{x})$ is the variance of dosage fluctuations about the mean value:

$$\sigma^2 = Var[d(\mathbf{x})] = \overline{d^2(\mathbf{x})} - \overline{d(\mathbf{x})}^2 = \overline{d'^2}(\mathbf{x}) \qquad (5)$$

HPAC also assumes that dosage fluctuations are described by a clip-normal distribution with parameters μ_G and σ_G

$$p_{CN}(d;\mu_G,\sigma_G) = \frac{1}{2}\left(1 - erf\left(\frac{\mu_G}{\sigma_G\sqrt{2}}\right)\right)\delta(d-0) + \frac{1}{\sigma_G\sqrt{2\pi}}\exp\left(-\frac{(d-\mu_G)^2}{2\sigma_G^2}\right), \quad d \geq 0 \qquad (6)$$

where *erf* is the error function and $\delta(d-0)$ denotes the Dirac delta function evaluated at $d = 0$, i.e., $\delta(d-0) = \begin{cases} 1 \text{ if } d = 0 \\ 0 \text{ otherwise} \end{cases}$

The predicted mean and variance of the dosage $(\mu,\sigma^2) = (\overline{d},\overline{d'^2})$ can be related to the parameters of the clip-normal distribution μ_G and σ_G by the following equations (Sykes et al., 2007):

$$\mu = \frac{\sigma_G}{\sqrt{2\pi}}\exp\left(-\frac{\mu_G^2}{2\sigma_G^2}\right) + \frac{\mu_G}{2}\left(1 + erf\left(\frac{\mu_G}{\sigma_G\sqrt{2}}\right)\right)$$
$$\sigma^2 = -\mu^2 + \frac{\sigma_G^2}{2}\left(1 + erf\left(\frac{\mu_G}{\sigma_G\sqrt{2}}\right)\right) + \mu_G\mu \qquad (7)$$

Equation 7 must be numerically inverted to obtain the clip-normal parameters μ_G and σ_G from the HPAC outputs $\overline{d}$ and $\overline{d'^2}$ (μ and σ^2).

Consequence Assessment Using HPAC's Ensemble-Mean Dosage

We now formally introduce an intuitive way of performing consequence assessment based on the ensemble-mean dosage alone. Let $\overline{d}_{\mathbf{x}}$ denote the mean dosage at any given location $\mathbf{x}$. For a prescribed dosage threshold l, define

$$H(d,l) = \begin{cases} 1 \text{ if } d > l \\ 0 \text{ otherwise} \end{cases} \qquad (8)$$

The function $H(\overline{d}_{\mathbf{x}},l)$ therefore indicates whether the mean dosage at a location $\mathbf{x}$ lies above threshold l. Thus, the area over which the mean dosage exceeds the threshold is

$$Area(\overline{\mathbf{d}},l) = \int_{\mathbf{x}} H(\overline{d}_{\mathbf{x}},l)d\mathbf{x} \qquad (9)$$

Similarly, given a population density $\rho(\mathbf{x})$, the number of casualties is

$$Cas(\overline{\mathbf{d}}) = \int_{\mathbf{x}} Cas(\overline{d}_{\mathbf{x}})\rho(\mathbf{x})d \qquad (10)$$

Consequence Assessment Using HPAC's Probabilistic Distribution of Dosages

Next we introduce a methodology to calculate the expected consequences using the probabilistic dosage distribution available in HPAC. For a specified location **x**, assume that individual turbulent realizations of the dosage are distributed according to a clip-normal distribution $p_{CN}(d;\mu_x,\sigma_x)$ given by Equation 6. Then

$$E[H(\bullet,l)] = \int_0^\infty H(\tau,l)\,p_{CN}(\tau;\mu_x,\sigma_x)\,d\tau = \int_l^\infty p_{CN}(\tau;\mu_x,\sigma_x)\,d\tau \quad (11)$$

Here $E[\bullet]$ denotes the statistical expectation with respect to the random variable describing the dosage distribution. We note that, in this formulation, Equation 11 is equivalent to calculating the probability that a randomly distributed dosage at a given location **x** exceeds some threshold value *l*. However, upon applying Equation 6, the right side of Equation 11 is equivalent to the integral of the the density function of the normal distribution from *l* to ∞ (when $l > 0$). For a normal distribution with mean μ_x and standard deviation σ_x, the cumulative density function $\Phi(\bullet;\mu_x,\sigma_x)$ can be computed as:

$$\Phi(d;\mu_x,\sigma_x) = \frac{1}{2}\left[1 + erf\left(\frac{d-\mu_x}{\sigma_x\sqrt{2}}\right)\right] \quad (12)$$

Thus,

$$E[Area(\bullet,l)] = E[H(\bullet,l)] = 1 - \Phi(l;\mu_x,\sigma_x) = \frac{1}{2}\left[1 - erf\left(\frac{l-\mu_x}{\sigma_x\sqrt{2}}\right)\right] \quad (13)$$

This expression gives the probability that the dosage will exceed some threshold value *l* at location **x**. Integrating over all locations x yields the expected (or average) area over which the dosage exceeds *l*:

$$< Area(l) >= \frac{1}{2}\int_{\mathbf{x}}\left[1 - erf\left(\frac{l-\mu_x}{\sigma_x\sqrt{2}}\right)\right]d\mathbf{x} \quad (14)$$

Starting with the expression in Equation 3 for casualties at a single location, the expected number of casualties at a location **x** that has a population density $p(\mathrm{x})$ can be calculated via numerical integration of

$$E[Cas(\bullet)] = \int_0^\infty Cas(\tau)\,p_{CN}(\tau;\mu_x,\sigma_x)\,\rho(\mathbf{x})\,d\tau \quad (15)$$

The expected casualties from the hazardous plume are:

$$< Cas >= \int_{\mathbf{x}}\int_0^\infty Cas(\tau)\,p_{CN}(\tau;\mu_x,\sigma_x)\,\rho(\mathbf{x})\,d\tau\,d\mathbf{x} \quad (16)$$

Brief Description of a Small-Scale Chemical Attack

In order to compare these consequence estimation methodologies, we simulated a notional small-scale chemical artillery attack of 18 individual artillery rounds impacting simultaneously within a 200-meter by 100-meter target box (Figure 1), with each round dispersing 1.6 kg of chemical agent. We created six sets of HPAC predictions using wind speeds of 5, 10, and 15 km/hr with the Pasquill-Gifford atmospheric stability categories of moderately stable (PG3) and slightly unstable (PG6), roughly corresponding to certain nighttime and daytime release conditions, respectively. We calculated hazard areas and numbers of casualties using the previously described methodologies. We also examined the "on target" hazard areas and casualties occurring only within the 200-meter-by-100-meter attack box. To better understand the effects

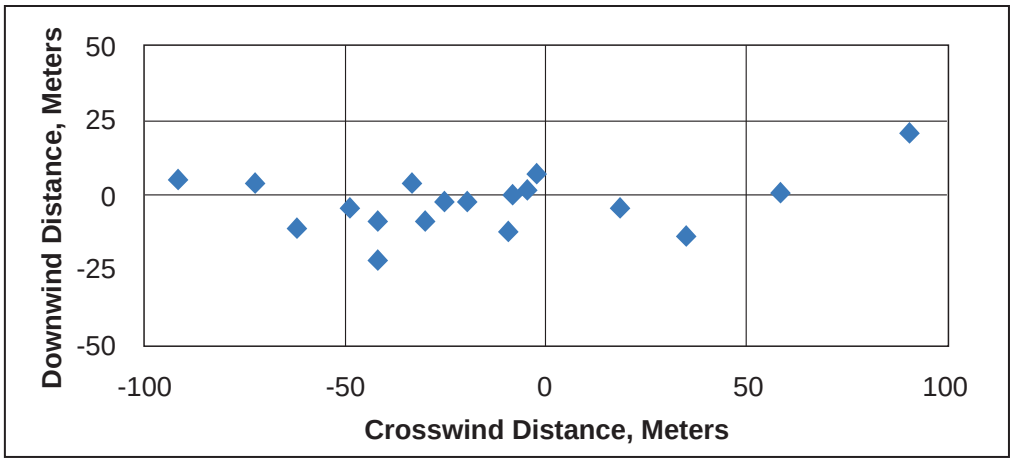


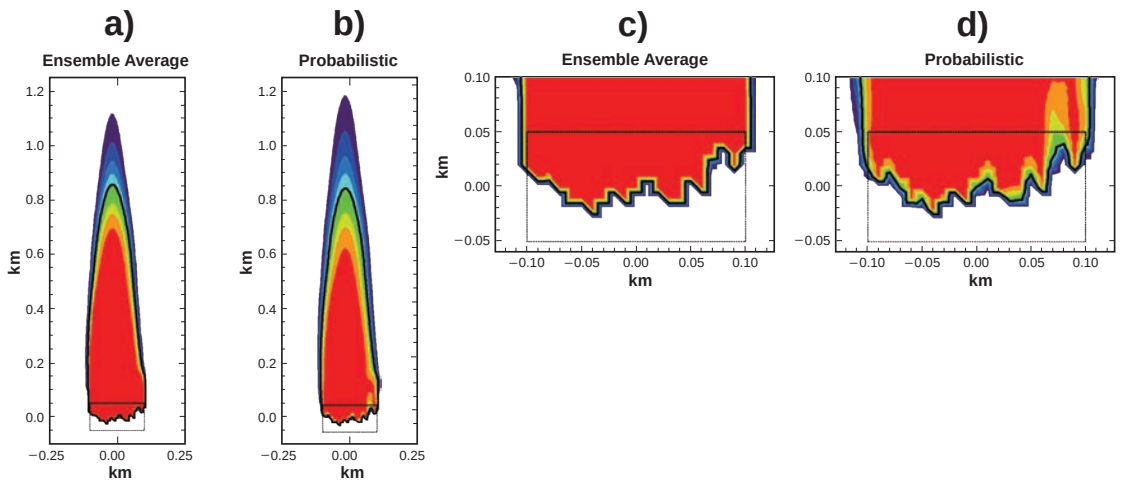
Figure 1. Relative Locations of 18 Individual Chemical Source Terms

of dosage threshold on hazard area calculations, we considered notional hazards occurring at seven different likelihoods of lethality: LCt_{99}, LCt_{90}, LCt_{50}, LCt_{5}, LCt_{1}, and $LCt_{0.1}$, where LCt_x ("lethal concentration x") is the concentration at which x% of the exposed population would die without medical intervention. The principal metric we used is the ratio of the expected hazard area or number of casualties estimated probabilistically from Equation 14 or 16 to the expected hazard area or number of casualties estimated from the ensemble-mean dosage plume using Equation 9 or 10.

Brief Summary of the Results

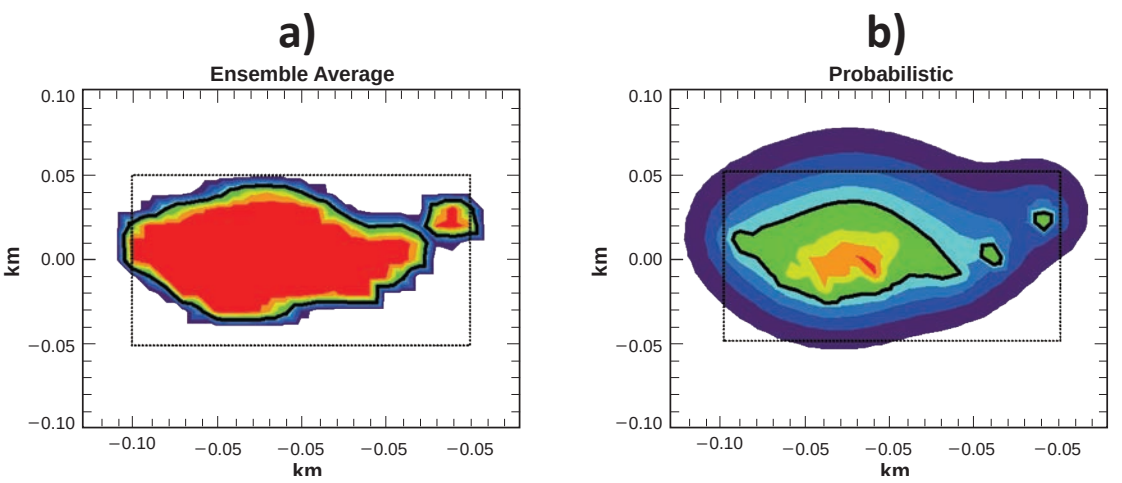
Figures 2 and 3 depict typical fractional lethality contours in the case of a moderately stable (PG6) or slightly unstable (PG3) atmosphere. Fractional casualties is the fraction of the exposed population that is expected to suffer casualties at the specified toxic endpoint (e.g., death). The thick black contour corresponds to a fractional lethality of 0.5, and the black dotted rectangle denotes the on-target attack box. In the case of moderately stable atmospheric conditions, the differences between the casualty contours generated using the two different methods are minor, especially when one considers the full extent of the contours (Figures 2a and 2b) instead of only the on-target attack box (Figures 2c and 2d). However, in the case of slightly unstable atmospheric conditions, the differences between the two methods of estimating casualties are significant (Figures 3a and 3b). These differences include both the locations at which casualties are expected to occur (larger areas for using the probabilistic dosage method than the ensemble-mean dosage method) and the number of casualties at individual locations (significantly larger at most locations using the ensemble-mean dosage method).

Figure 4 depicts the ratios of expected casualties based on probabilistic dosages to casualties based on ensemble-averaged dosages for the two atmospheric stability categories and three wind speeds considered in this analysis. For moderately stable atmospheric



Panel a) depicts contours calculated from the ensemble-averaged dosage, panel b) depicts contours calculated from a clip-normal probabilistic dosage distribution, and panels c) and d) zoom in on the on-target attack box depicted in panels a) and b).

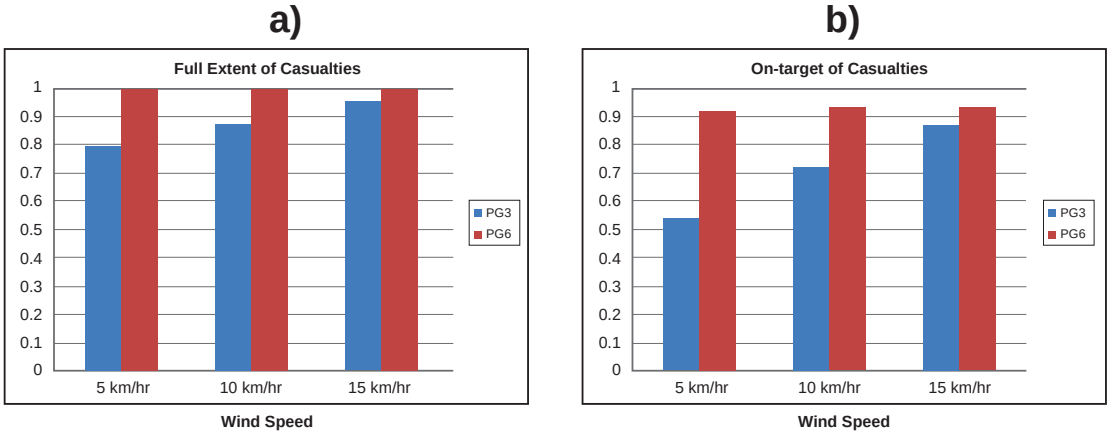
Figure 2. Fractional Lethality Contours for a Moderately Stable Atmosphere (PG6) and a Wind Speed of 10 km/hr



Panel a) depicts contours calculated from the ensemble-averaged dosage, and panel b) depicts contours calculated from a clip-normal probabilistic dosage distribution.

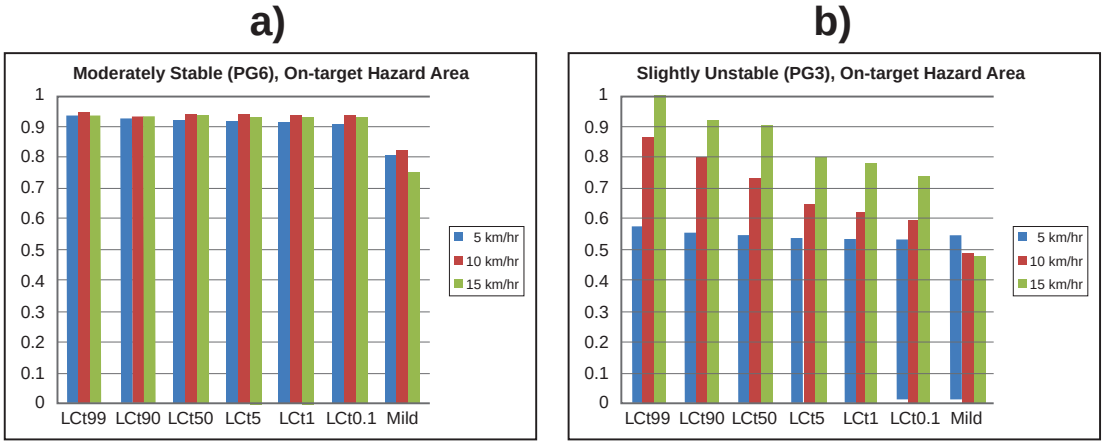
Figure 3. Fractional Lethality Contours for a Slightly Unstable Atmosphere (PG3) and a Wind Speed of 10 km/hr

conditions, the casualty ratio is close to 1, indicating that both methods of estimating casualties produce similar results. However, when the atmospheric conditions are slightly unstable, varying wind speed yields casualty ratio variation from 0.55 to 0.94, indicating that the ensemble-mean dosage method of calculating casualties can result in significantly higher casualty estimates than the probabilistic dosage method.



In panel a), casualties are calculated over full extent of the plume, and panel b) casualties are calculated only within the on-target attack box.

Figure 4. Ratio of Expected Lethalities



Panel a) correspond to moderately stable atmospheric conditions (PG6) and panel b) correspond to slightly unstable atmospheric conditions (PG3).

Figure 5. Ratios of the Expected Hazard Areas

Figure 5 depicts the ratios of the hazard area calculated based on probabilistic dosages to the hazard area calculated based on the ensemble-mean dosage for two atmospheric stability categories, three wind speeds, and seven notional toxic effects levels for on-target attacks. For moderately stable atmospheric conditions, the two methods of consequence assessment yield similar values (Figure 5a). In the case of a slightly unstable atmosphere (Figure 5b), there is a greater spread in the hazard area ratios that depends on the level of effects and the wind speed with potential difference up to a factor of two in the size of the predicted hazard area.

Conclusions

We simulated a small-scale chemical weapons attack to investigate the implications of using two methods

for dosage-based consequence assessment: one using the HPAC model's probabilistic predictions of agent dosage, and one using HPAC's ensemble-mean predictions of dosage. We note that the ensemble-mean dosage method is the usual method applied in the consequence assessment community, whereas the probabilistic dosage method has not been widely adopted.

Our main conclusion is that care should be exercised when using an ensemble-mean dosage plume to calculate the consequences from an atmospheric release of toxic materials. We found that at least for our single small-scale chemical attack scenario considered under a few different meteorological conditions, the two methods of dosage-based consequence assessment yielded similar results in the case of moderately stable atmospheric conditions, but dissimilar results in the case of slightly unstable atmospheric conditions. In the latter case, depending on wind speed and the size of the targeted area, an over-prediction of consequences of up to a factor of two is possible when using the commonplace ensemble-mean dosage method. Additionally, the spatial distribution of casualties and hazard areas could differ significantly between these two methods of performing consequence assessment.

We note a significant conceptual difference between these two approaches to dosage-based consequence assessment. AT&D models that predict ensemble-mean dosages have the advantage of being able to produce a plot of the "average" plume. Since the toxicity equations that map dosages to adverse health effects are nonlinear, consequence estimates based on these ensemble-averaged plumes do not represent ensemble-averaged casualties or hazard areas. On the other hand, AT&D models that are capable of producing probabilistic dosage distributions can be used to calculate average casualties or hazard areas correctly, but the probabilistic description does not readily lend itself to producing easy-to-interpret plots of the location of the hazard. Moreover, it might be possible to calculate uncertainties associated with the consequences of the attack such as variance of the casualty estimate.

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