THE USE OF PROBABILISTIC PLUME PREDICTIONS FOR THE CONSEQUENCE ASSESSMENT OF ATMOSPHERIC RELEASES OF HAZARDOUS MATERIALS

Nathan Platt[1], William Ross Kimball II[2], Jeffry T. Urban[1]

[1]Institute for Defense Analyses, Alexandria, Virginia, USA
[2]Johns Hopkins University, Baltimore, Maryland, USA

Abstract: The most common way for an atmospheric transport and dispersion (AT&D) modelling system to calculate the toxic effects of a chemical weapons exposure is based on the total inhaled dose, according to Haber's Law of toxicity. The majority of AT&D models presently used for consequence assessment predict only a "mean" plume that approximates the ensemble average over many possible plume realizations. Typically, consequence assessments are performed by directly applying Haber's Law to the predicted ensemble-mean dosage to estimate hazard areas or casualties. In reality, personnel are never exposed to a "mean" plume, but to one of many possible individual statistical realizations of a plume. Therefore, a potential disconnect may occur between the output of common AT&D modelling systems and the consequence metrics that are of interest to decision-makers. Some AT&D models not only predict the ensemble-mean dosage, but also the variance about the mean making it possible to construct a fully-probabilistic dosage plume that provides consistent estimates of the consequences along with estimates of the statistical uncertainty around the expected values. We demonstrate and compare these two consequence assessment methodologies using HPAC's simulations of a small-scale chemical artillery attack.

Key words: *casualty assessment, consequence assessment, Haber's law, ensemble averaged plume, probabilistic consequence assessment, Hazard Prediction and Assessment Capability, HPAC***.**

INTRODUCTION

Atmospheric transport and dispersion (AT&D) models play an important role in the U.S. Department of Defense (DoD) due to the threat of battlefield or terrorist use of chemical and biological weapons. There is a need to accurately model the consequences expected from the intentional or accidental release of hazardous materials into the atmosphere. Casualty estimation requires toxicological models that relate chemical exposures to the toxic effects on humans. A common assumption is that toxic effects are a function 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 $C(\mathbf{x})$ (Eq. 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, a simple conceptual extension of Haber's Law to the case of a dosage $d(\mathbf{x})$ derived from a time-varying concentration $c(\mathbf{x},t)$ (Eq. 2) is applied quite prevalently, although it is not based on empirical data.

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

For any given level of exposure, there is a need to estimate the level of toxic effects. The typical toxicological response model used for consequence assessments 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, and is shown in Eq. 3.

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

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, etc.) in 50% of the population.

The majority of AT&D models presently used for consequence assessment predict only a "mean" plume that approximates the ensemble average over a large number of plume realizations. Typically, consequence assessments are performed by using ensemble-mean dosage predictions from these models to calculate either the expected location of a hazardous area or the expected number of casualties. 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 modelling system maintained and distributed by the U.S. Defense Threat Reduction Agency. SCIPUFF is a Lagrangian Gaussian puff dispersion model that, in addition to calculating mean dosage, also calculates dosage variance. If $d(\mathbf{x})$ represents the dosage field for a single turbulent realization of the toxic plume, this dosage field can be decomposed as

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

where the overbar denotes the ensemble mean and the prime denotes a realization of the turbulent fluctuation about the mean. 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 $\overline{d'^2(\mathbf{x})}$ can be associated with the variance of dosage fluctuations about the mean value:

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

In addition, HPAC assumes that dosage fluctuations can be described by a clip-normal distribution with parameters μ_G and σ_G

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

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):

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

In order to develop a probabilistic description of casualties using the assumption of clip-normally distributed dosages, Eq. 7 must be 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). Since these equations cannot be inverted analytically, we used a numerical implementation of the multi-dimensional Newton's method for root-finding (Press et. al., 1992).

Consequence assessments usually use one or both of two types of toxicity-based metric to characterize the adverse health effects that may be associated with a release of a hazardous material: estimates of the location of the area enclosed within a hazardous zone given some effects threshold such as 1% casualties (Eff_{01}) or mild effects (Eff_{mild}) that might correspond to exposed personnel experiencing blurry vision or watery eyes, or the total number of casualties or the spatial distribution of casualties.

CASUALTY ASSESSMENT USING HPAC'S ENSEMBLE-MEAN DOSAGE

In this section, we formally introduce intuitive way of doing consequence assessment based on ensemble-mean dosage alone. Let $\overline{d}_{\mathbf{x}}$ denote mean dosage at any given location **x**. For HPAC, please note that $\overline{d}_{\mathbf{x}}$ is the true mean of the clip-normal distribution provided in the output sampler file – it is not a converted equivalent mean μ_G of the normal distribution that was used previously. For a prescribed dosage threshold *l*, define

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

We note that this function is related to the Heaviside step function, whose value is zero for negative arguments and one for positive arguments, by choosing the argument of the Heaviside function to be *d* - *l*. Then, for any location **x**, whether or not this location lies above threshold *l* is determine by whether or not $\overline{d}_{\mathbf{x}} > l$, i.e. when

$$H(\overline{d}_{\mathbf{x}}, l) = 1 \tag{9}$$

Thus, area above threshold is determined by

$$Area(\overline{d}) = \int_{\mathbf{x}} H(\overline{d}_{\mathbf{x}}, l)\, d\mathbf{x} \tag{10}$$

Similarly, casualties are calculated by

$$Cas(\overline{d}) = \int_{\mathbf{x}} Cas(\overline{d}_{\mathbf{x}})\rho(\mathbf{x})\, d\mathbf{x} \tag{11}$$

CASUALTY ASSESSMENT USING HPAC'S PROBABILISTIC DISTRIBUTION OF DOSAGES

In this section we expand consequence assessment methodology from the previous section to calculate expected consequences resulting from the probabilistic dosage distribution description available in HPAC. For a specified location **x**, assume that individual turbulent realizations of the dosage are distributed according to a clip-normal distribution $p_{CN}(d;\ \mu_{\mathbf{x}},\sigma_{\mathbf{x}})$ given by Eq. 6. As described earlier, $(\mu_{\mathbf{x}},\sigma_{\mathbf{x}})$ are the parameters of the normal distribution that defines the clip-normal distribution of dosages, which we calculated using Newton's root finding method from HPAC's physics-based estimates of the mean and standard deviation of the dosage fluctuations. Then

$$E\left[H(\bullet,l)\right]=\int_0^\infty H(\tau,l)\,p_{CN}(\tau;\mu_{\mathbf{x}},\sigma_{\mathbf{x}})d\tau=\int_l^\infty p_{CN}(\tau;\mu_{\mathbf{x}},\sigma_{\mathbf{x}})d\tau \tag{12}$$

Here $E[\bullet]$ denotes the statistical expectation with respect to the random variable describing the dosage distribution. We note that in this formulation, Eq. 12 is equivalent to calculating probability that a randomly distributed dosage at a given location **x** exceeds some threshold value *l*. However, upon applying Eq. 6 , the right side is equivalent to integrating the density function of the normal distribution from *l* to ∞ (when $l < 0$). For a normal distribution with mean $\mu_{\mathbf{x}}$ and sigma $\sigma_{\mathbf{x}}$, the cumulative density function $\Phi(\bullet;\mu_{\mathbf{x}},\sigma_{\mathbf{x}})$ can be computed as:

$$\Phi(d;\mu_{\mathbf{x}},\sigma_{\mathbf{x}})=\frac{1}{2}\left[1+erf\left(\frac{d-\mu_{\mathbf{x}}}{\sigma_{\mathbf{x}}\sqrt{2}}\right)\right] \tag{13}$$

Thus,

$$E\left[H(\bullet,l)\right]=1-\Phi(l;\mu_{\mathbf{x}},\sigma_{\mathbf{x}})=\frac{1}{2}\left[1-erf\left(\frac{l-\mu_{\mathbf{x}}}{\sigma_{\mathbf{x}}\sqrt{2}}\right)\right] \tag{14}$$

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*:

$$<Area(l)>=\frac{1}{2}\int_{\mathbf{x}}\left[1-erf\left(\frac{l-\mu_{\mathbf{x}}}{\sigma_{\mathbf{x}}\sqrt{2}}\right)\right]d\mathbf{x} \tag{15}$$

Using a similar procedure starting with the expression in Eq. 3 for casualties at a single point, the expected number of casualties at a location **x** with a given population density $\rho(\mathbf{x})$ can be calculated via numerical integration of

$$E\left[Cas(\bullet)\right]=\int_0^\infty Cas(\tau)\,p_{CN}(\tau;\mu_{\mathbf{x}},\sigma_{\mathbf{x}})\rho(\mathbf{x})d\tau \tag{16}$$

and expected casualties due to a given dosage distribution $d_{\mathbf{x}}$ at location **x** and population density $\rho(\mathbf{x})$ can be determined via

$$<Cas>=\int_{\mathbf{x}}\int_0^\infty Cas(\tau)\,p_{CN}(\tau;\mu_{\mathbf{x}},\sigma_{\mathbf{x}})\rho(\mathbf{x})d\tau d\mathbf{x} \tag{17}$$

BRIEF DESCRIPTION OF A SMALL SCALE CHEMICAL ATTACK

In order to compare consequence estimates (the size of hazardous areas or the number of casualties) based on HPAC probabilistic dosage predictions with consequence estimates based on HPAC ensemble-mean dosage predictions, we simulated a notional small-scale chemical artillery attack. This attack consists of the simultaneous impact of 18 individual artillery rounds within a 200-meter by 100-meter target box with each round dispersing 1.6 kg of chemical agent. For the AT&D calculations we assume a surface roughness corresponding to urban terrain, along with a uniform population density. 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 total hazard areas and casualties and also examined the "on target" hazard areas and casualties occurring only within the 200-meter by 100-meter attack box. Typical hazard area calculations involve dosage thresholds that might represent either a low-level exposure that causes mild effects such as blurry vision or watery eyes, or the threshold at which lethality may begin to be expected (such as dosages that are expected to cause 1% or 0.1% lethality in the affected population). However, to better understand the effects of dosage threshold on hazard area calculations, we considered notional hazards occurring at seven different levels that included not only mild effects but also several 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 main quantitative metric used in this work is the ratio of the expected hazard area or number of casualties estimated probabilistically from Eq. 15 or 16 to the expected hazard area or number of casualties estimated from the ensemble-mean dosage plume using Eq. 10 or 11.

BRIEF SUMMARY OF THE RESULTS

Fig. 1 and 2 depict typical fractional casualties contours obtained from HPAC simulations of the attack in the case of a moderately stable (PG6) or slightly unstable (PG3) atmosphere. Fractional casualties refer to the fraction of the exposed population that is expected to incur casualties at the specified toxic endpoint (e.g., death). The contour increment is 0.1 and the contours start at 0.1 (10% lethality). Thick black contour corresponds to fractional lethality of 0.5 (50%) and the black dotted rectangle denotes the on-target attack box. In the case of moderately-stable atmospheric conditions (PG6) the differences between the casualties contours generated using

the two different methods (probabilistic dosage and ensemble-mean dosage) are minor, especially when one considers the full extent of the contours (Fig. 1a and 1b) instead of only the on-target attack box (Fig. 1c and 1d). In the case of slightly unstable atmospheric conditions (PG3) the differences between the two methods of estimating casualties are significant, in contrast to the moderately-stable case. 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).

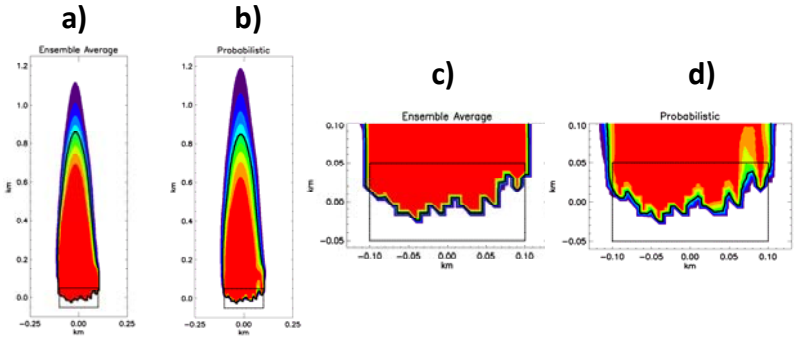

Fig.1: Fractional lethality contours for a moderately stable atmosphere (Pasquill Gifford Category 6). Panel a) depicts contours calculated from the ensemble-averaged dosage, panel b) depict contours calculated from a clip-normal probabilistic dosage distribution, and panels c) and d) zooming on the on-target attack box depicted in panels a) and b) (respectively).

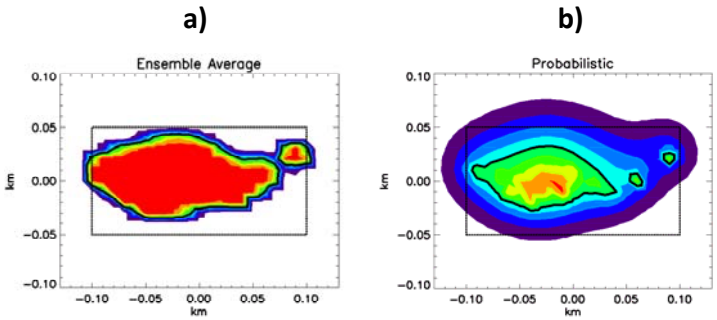

Fig.2: Fractional lethality contours for a slightly unstable atmosphere (PasquillGifford Category 3). Panel a) depict contours calculated from the ensemble-averaged dosage and panel b) depict contours calculated from a clip-normal probabilistic dosage distribution.

Fig. 3 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 study. For moderately stable atmospheric conditions the casualty ratio is approximately 1 when considering the full plume and approximately 0.93 for the on-target attacks, 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 0.8 to 0.94 when considering the full plume and from 0.55 to 0.88 in the on-target attack box indicating that the ensemble-mean dosage method of calculating casualties can result in significantly higher casualty estimates than the probabilistic dosage method when considering toxic effects in the targeted region.

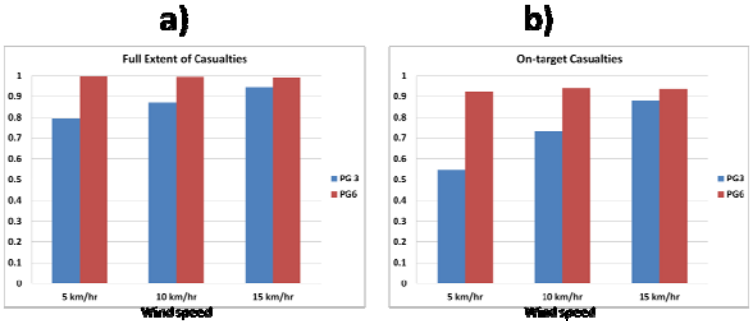

Fig.3: Ratio of expected lethalities based on probabilistic dosage predictions to expected casualties based on ensemble-mean dosage predictions. In panel a) casualties are calculated over full extent of the plume and panel b) casualties are calculated only within the on-target attack box.

Fig. 4 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 (Fig. 4a). In the case of a slightly unstable (PG3) atmosphere (Fig. 4b), 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.

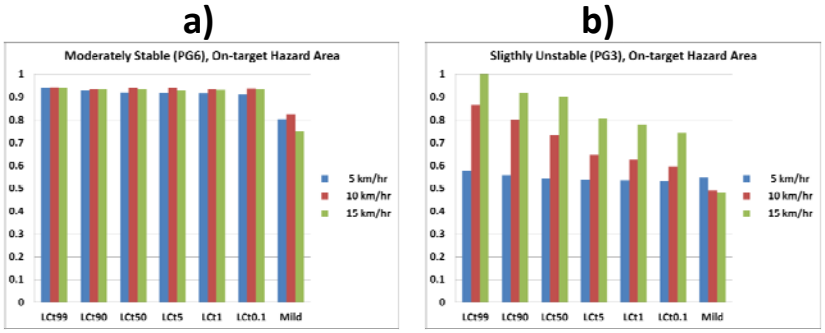

Fig.4: Ratios of the expected hazard area based on probabilistic dosages to the expected hazard area based on ensemble-mean dosages. Panel a) correspond to moderately stable atmospheric conditions (PG6) and panel b)) correspond to slightly unstable atmospheric conditions (PG3).

CONCLUSIONS

In this paper 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 (along with an additional assumption about the form of the dosage distribution across turbulent realizations of the plume), 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 some care should be exercised when using an ensemble-mean dosage plume to calculate the consequences to human health 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. Additionally, it might be possible to calculate uncertainties associated with the consequences of the attack such as variance of the casualty estimate.

Acknowledgements: This effort was supported by the Defense Threat Reduction Agency with Dr. John Hannan as the project monitor. The authors would like to thank Dr. Don Lloyd from the Institute for Defense Analyses for fruitful discussions regarding this work and for providing parameters for the small-scale chemical attack. The views expressed in this paper are solely those of the authors.

REFERENCES

Press, W.H., Teukolsky, S.A., Vetterling, W.T. and B.P. Flannery, 1992: Numerical Recipes in C: The Art of Scientific Computing (Second Edition), Cambridge University Press.

Sykes, R.I., Parker, S.F., Henn, D.S., and B. Chowdhury, 2007: SCIPUFF Version 2.3 Technical Documentation, L-3 Titan Technical Report.