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USE OF THE ENSEMBLE-MEAN PLUME VERSUS INDIVIDUAL PLUME REALIZATIONS FOR TOXIC LOAD MODELING

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Abstract: The most common way for an atmospheric transport and dispersion (AT&D) model to calculate toxic effects is based on the total inhaled dose. These effects are independent of the manner in which this dose was accumulated. But for many chemicals, it has been observed that the time dependence of the concentration is important. Toxic load modelling tries to account for this by utilizing the toxic load exponent. While the experimental data supporting toxic load modelling were derived using a rectangular pulse concentration exposure profiles, the actual exposures from hazardous plumes are temporally highly variable. There are several proposed generalizations of the toxic load model to the case of time-varying exposure profiles, none of which have been validated using animal experiments. The majority of present-day AT&D models used for consequence assessment estimate a "mean" plume that approximates the ensemble average over a large number of plume realizations. The few models that utilize the toxic load model apply it using this mean plume. We have obtained a high resolution (in space and time) set of VTHREAT predictions that contains 20 plume realizations for a continuous release of a neutral-buoyancy tracer gas over flat terrain under stable atmospheric conditions. We use this data set for comparing toxic load calculations based on a "mean" plume with calculations based on individual plume realizations in order to assess the potential effect on casualty estimation.

Key words: *casualty assessment, consequence assessment, Haber's law, toxic load modelling, ensemble averaged plume, VTHREAT.*

INTRODUCTION

There is anecdotal evidence that atmospheric transport and dispersion (AT&D) models greatly over-predict the consequences of large scale toxic industrial chemical releases (Urban et al., 2010 and Sommerville et al., 2009). This evidence is largely based on a comparison between the observed locations of human or animal casualties (or lack thereof) resulting from chlorine rail car accidents and the hazard area for lethal effects derived from AT&D model predictions. There are a number of potential reason for these discrepancies, which include: (1) inaccurate descriptions of the input parameters needed to run AT&D models, such as source term descriptions and meteorology; (2) the potential inability of AT&D models to capture some important features associated with the propagation of a large volume of dense vapour; and (3) inaccurate consequence estimation models, including potential inaccuracies in the in toxicity parameters or in the toxicity models used to estimate toxic inhalation effects. This work concentrates on the consequence estimation methodology, specifically on a toxic load modelling of the assessment of casualties.

The most common way for an AT&D model to calculate toxic effects is based on the total inhaled dose. These effects are independent of the manner in which this dose was accumulated (i.e., they are independent of the exposure history). But for many chemicals, it has been observed that the time dependence of the exposure is important – for instance, inhaling a dose of chlorine over a short period of time has much stronger effects than inhaling the same dose over an extended period of time (ten Berge et al., 1986 and Sommerville et al., 2009). Toxic load modelling tries to account for this effect by utilizing the toxic load exponent n (which is, for example, approximately equal to 2.75 for chlorine) (Sommerville et al., 2009). While the experimental data supporting toxic load modelling were derived using concentration exposure profiles in the form of a rectangular pulse, the actual exposures from hazardous plumes are not well-described by rectangular pulses. There are several proposed generalizations of the toxic load model to the case of time-varying concentration, none of which have been validated using animal experiments. In this work, a total of four toxic load models are considered that cover the full spectrum of conservatism in casualty and hazard area estimation.

The majority of AT&D models presently used for consequence assessment predict a "mean" plume that approximates the ensemble average over a large number of plume realizations. In a number of studies, toxic load modelling is applied to the concentration output of these models to produce casualty estimates. Additionally, the few AT&D models that apply toxic load modelling internally use the ensemble average plume (some models may also include statistical estimates of the variance of the ensemble average, e.g. Sykes et al., 2007). By its definition, the "mean" plume "smears out", in both time and space, the high concentration regimes that would be expected within individual plume realizations. The question arises whether the casualties estimated from the "mean plume" could differ from the mean of the casualties estimated from individual plume realizations when using toxicity models that depend on the time history of the exposure, such as toxic load models.

The National Center for Atmospheric Research (NCAR) Virtual Threat Response Emulation Test Bed (VTHREAT) modelling system is a suite of models designed to provide a virtual environment for meteorological modelling and AT&D modelling. It includes an Eulerian semi-Lagrangian model for geophysical flows (EULAG) that utilizes a Large Eddy Simulation (LES) numerical technique coupled with a Lagrangian Particle Dispersion Model (LPDM) (Bieberbach et al., 2010). A key feature of VTHREAT is its potential to produce realistic, statistically representative hazardous materials plumes that include turbulence-induced fluctuating and meandering components. VTHREAT actually predicts individual realizations of the plume and not a "mean" plume.

We have obtained a high resolution (in space and time) set of predictions that contains 20 plume realizations for a continuous release of a neutral-buoyancy tracer gas over flat terrain under stable atmospheric conditions. This data set is an ideal

candidate for comparing toxic load calculations based on a "mean" plume with calculations based on individual plume realizations in order to assess the potential effect on casualty estimation. Figure 1 depicts snapshots at 500 seconds from the start of the continuous release of a single realization of the concentration field at 5 meters above ground level (left panel = 1-second time resolution, right panel = point-to-point ensemble-averaging over 20 realizations followed by 60-second running-window time average).

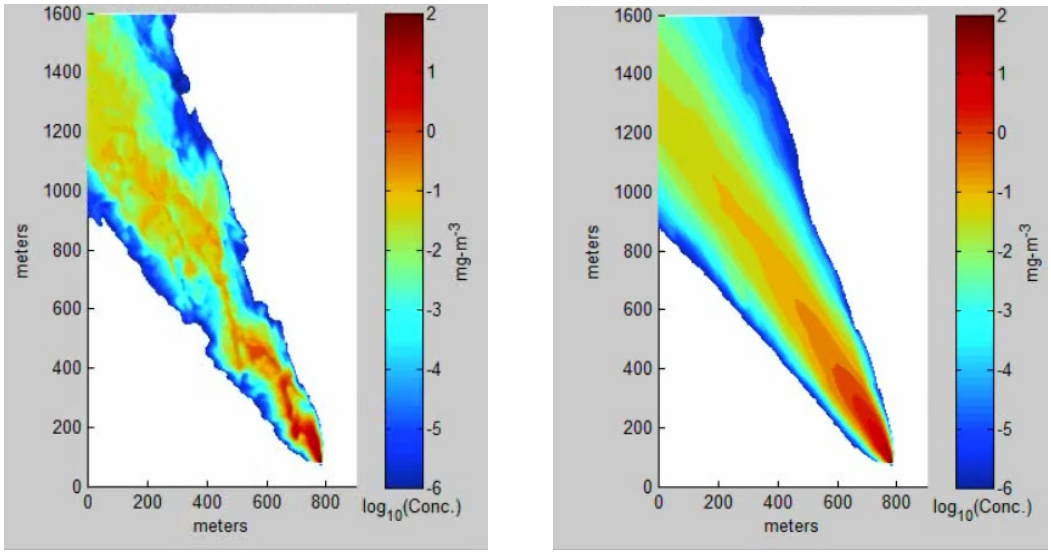

Fig.1: Example VTHREAT-simulated concentration field for an individual realization (on the left) and ensemble-averaged plume (on the right).

HABER'S LAW AND TOXIC LOAD MODELING

Different models have been proposed to relate a chemical concentration exposure profile to the toxic effect on humans. A common assumption is that toxic effects are a function of only the total inhaled dosage. This relationship between exposure and toxic response is called Haber's law, which can be written as follows:

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

where $D(x)$ denotes the dosage at a location x and $C(x)$ is a constant concentration to which a subject located at point x is exposed over a duration T. According to Haber's law, the toxic effect are identical as long as the total dosage is the same, regardless of whether the dosage is delivered via a long exposure to a low concentration or a short exposure to a high concentration. While the original Haber's law was defined for constant concentration only, a simple extension of Haber's law to a non-steady time-varying concentration $c(x,t)$ is quite prevalent (Sommerville et al., 2006):

$$D(\mathbf{x}) = \int c(\mathbf{x},t)dt \qquad (2)$$

In this formulation, the limits of integration are irrelevant as long as they capture the entire passage of the hazardous plume at spatial location x. We note that when Haber's Law is assumed time-varying concentration, toxic effects are independent of the temporal history in which the dosage is accumulated.

For any given level of exposure, there is a need to estimate effects of such an exposure. While individual subjects might respond differently to the same dosage exposure, it is possible to use simple probabilistic notions to characterize overall subject group response when exposed to specific dosage – for instance what is the average number of healthy young soldiers that would be incapacitated when exposed to a prescribed dosage of a particular chemical. The typical model for consequence assessment used to estimate toxicological effects is a probit model based on a log-normal distribution described by two-parameters: the median effective dosage Eff_{50} and the probit slope. Eff_{50} corresponds to the dosage that is required to achieve a certain effect (e.g., death, incapacitation, etc.) in 50% of the population. To determine Eff_{50} and the probit slope, one typically needs to perform animal experiments to determine the dosage at which the specified toxicological effects occur; these results are then extrapolated to the human population. Typical studies involve exposing a number of animal subjects in a sealed chamber to constant concentrations of a toxic chemical over different time intervals and recording the fraction of the population that shows particular toxic effects.

Early in the study of chemical toxicity it was observed that Haber's law does not hold for all chemical agents, including several chemical warfare agents. Some authors have suggested that for these chemicals the population response is better described by a log-normal function of the "toxic load" than of the dosage, where the toxic load is defined as:

$$\begin{aligned} TL(\mathbf{x}) &= C^n(\mathbf{x})T \\ &= (C(\mathbf{x})T)^n T^{1-n} \qquad (3) \\ &= D^n(\mathbf{x})T^{1-n} \end{aligned}$$

Here, n is the "toxic load exponent", which, like the other toxicity parameters, is determined by fitting the available experimental exposure-response data. If $n > 1$, an exposure to a short-duration but high-concentration pulse produces stronger toxic effects than an exposure to a long-duration but low-concentration pulse. The toxic load model reduces to Haber's law when $n = 1$. As is the case with Haber's law, the toxic load model requires two additional parameters to estimate the fraction of the population exhibiting a particular toxic effect (e.g., death, incapacitation, etc.), such as the "median effective toxic load" and the corresponding probit slope. We note that the toxicity parameters associated with the use of a toxic load model may not equal the ones that apply when Haber's Law is assumed.

As is the case for Haber's law, the experimental basis for the toxic load model is derived based on constant concentration exposure only. In actuality, real-life exposures may vary in time. In addition, even simple AT&D models used in consequence assessment today produce time-varying concentration profiles. Thus, there is a need to extend the toxic load model described in Eq. 3 to non-steady exposures. Several such extensions have been proposed, but none have been validated experimentally.

In this paper we consider four different toxic load model (TLM) extensions for temporally non-constant concentration fields: Average Concentration TLM (Hilderman et al., 1999), Integrated Concentration TLM (ten Berge and van Heemst, 1983), Concentration Intensity TLM (Sykes et al., 2007) and Peak Concentration TLM (Stage, 2004) defined below. For further details please consult Platt et al., 2011.

$$TL_{AverConc}(\mathbf{x}) = \left(\frac{\int c(\mathbf{x},t)dt}{T} \right)^n T \qquad (4)$$

$$TL_{Integrated.}(\mathbf{x}) = \int c^n(\mathbf{x},t)dt \qquad (5)$$

$$T_{ConcIntens}(\mathbf{x}) = \frac{(\int c(\mathbf{x},t)dt)^2}{\int c^2(\mathbf{x},t)dt} \qquad (6)$$

$$TL_{PeakConc}(\mathbf{x}) = \frac{\int c(\mathbf{x},t)dt}{c_{Peak}^{1-n}(\mathbf{x})} \qquad (7)$$

Here, $c(\mathbf{x},t)$ denotes concentration at spatial location $\mathbf{x}$ and time t, T denotes actual plume duration at a give spatial location, c_{peak} denotes maximum concentration obtained at a given location, and n denotes toxic load exponent.

We note that when the toxic load exponent n equals 1, all of the aforementioned toxic load models reduce to Haber's law where exposure is a function of the total inhale dose only. It should be noted that for three of the toxic load models (Integrated Concentration, Concentration Intensity and Peak Concentration) it may be necessary to evaluate the toxic load using a concentration $c(\mathbf{x},t)$ that is time-averaged over a fast timescale to remove high-frequency concentration fluctuations. From a physiological perspective, it is unlikely that high-frequency concentration fluctuations that occur on a timescale faster than the time it takes to take a single breath of air would have a significant impact on human toxicity. Therefore, it may be necessary to apply a time-averaging of the concentration time series over a timescale on order of at least few seconds before calculating the toxic load integrals.

COMPARISON METRICS

For each individual plume realization provided by VTHREAT we calculated the toxic load at each location in the concentration field using each of the four toxic load models discussed previously. Each of these toxic load fields can be considered as representing the spatial distribution of toxic loads that could be delivered to a population in a real-world event. We also calculated the toxic load at each location using the ensemble-averaged concentration field directly. This toxic load field is intended to represent the distribution of toxic loads that might be predicted by a desktop AT&D model (such as a Gaussian plume or puff model). The following procedure was established to define a comparison metric: (1) choose a threshold toxic load value, (2) determine the area (in m^2) of the toxic load field that exceeds the threshold value at a given height above ground level, (3) repeat this process for a predetermined set of threshold toxic load values, (4) apply this process to the toxic load field calculated from the concentration field from each individual realization of a release, and (5) apply this process to the toxic load field calculated from the ensemble-average concentration field. Our metrics include not only the area-above-threshold values calculated for individual release realizations, but also the ratio of the area-above-threshold for each realization to the area-above-threshold for the toxic load calculated from the ensemble mean concentration. This ratio is a dimensionless quantity.

BRIEF SUMMARY OF THE RESULTS

Three different toxic load exponents n = 1, 1.5 and 2.75 were used to calculate the two "area-above-threshold" metrics described previously for each of the four toxic load models. These values span potential range of toxic load exponents for the chemical warfare agents and toxic industrial chemicals. For brevity we will present results for n = 2.75 only. For further details please see Platt et al., 2011. Figure 2 shows the areas-above-threshold as a function of the toxic load threshold level. The "realization mean", denoted by black circles, corresponds to the average of the area values taken over the 20 individual realizations (ensemble members). Likewise, the "realization maximum" (maximum area observed among the 20 realizations) is denoted by light green diamonds and the "realization minimum" is denoted by light blue squares. The vertical black line

denotes the span over which 90% (18 of 20) of the areas-above-threshold fall. The area-above-threshold values for the toxic load field calculated from the ensemble mean concentration are denoted by brown pluses. Panel a) shows results from the Average Concentration TLM, panel b) shows results from the Integrated Concentration TLM, panel c) shows results from the Peak Concentration TLM, and panel d) shows results from the Concentration Intensity TLM. Figure 3 is the same as Figure 2 except the individual areas-above-threshold have been normalized by dividing them by the area-above threshold for the toxic load field calculated from the ensemble mean concentration field. With the possible exception of the Average Concentration toxic load model, all realizations have a significantly larger toxic load area than the corresponding toxic load area calculated from the ensemble average concentration. Additionally, at the higher toxic load thresholds, both the Integrated Concentration and Concentration Intensity TLMs significantly under-predict hazard areas (by up to a factor of 6) when the toxic load calculated from the ensemble average concentration is used compared to either the hazard areas calculated from individual realizations or to the average of hazard areas calculated from individual plume realizations.

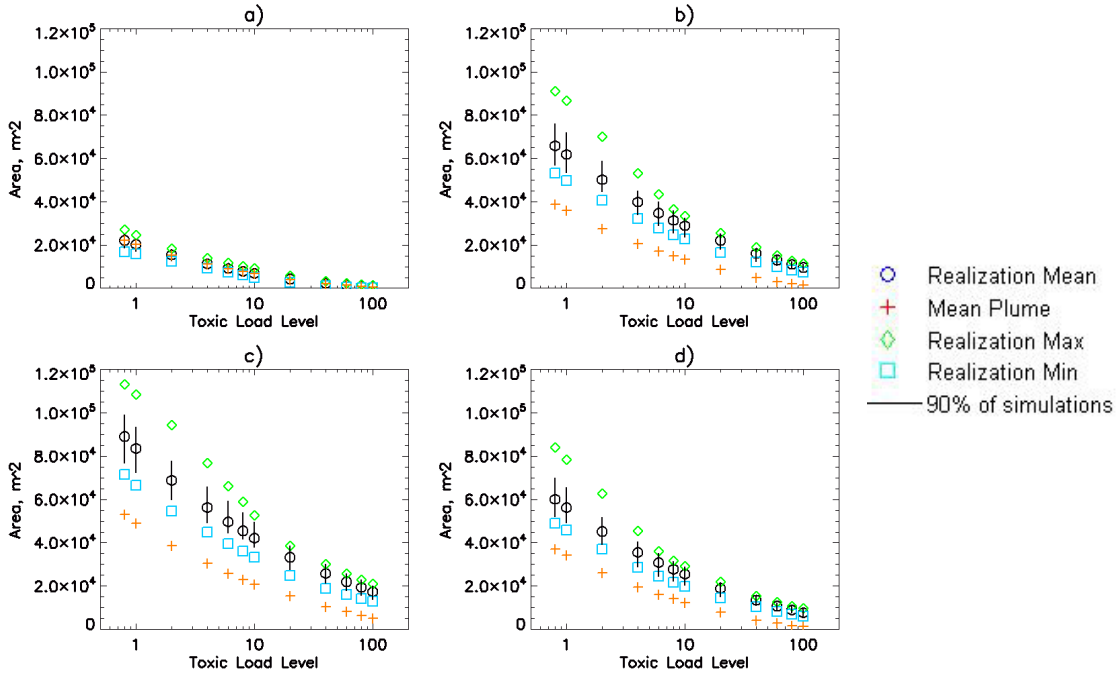

Fig.2: Area exceeding a threshold toxic load as a function of the threshold level for toxic load exponent n = 2.75.

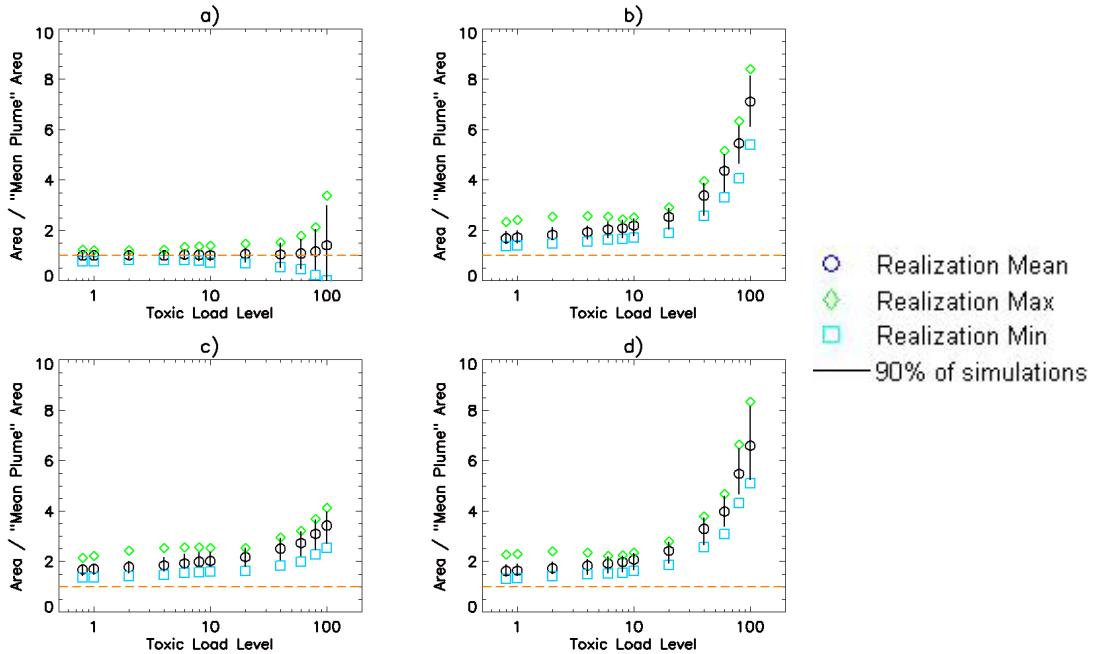

Fig.3: Ratio of the area exceeding a threshold toxic load for individual plume realizations to the area exceeding the threshold for the estimated ensemble mean plume as a function of the threshold level for toxic load exponent n = 2.75

CONCLUSIONS

In this paper we briefly investigated the potential effects of the choice of toxic load model and the use of ensemble-average plumes derived from AT&D models in place of individual plume realizations on the estimation of the toxic effects resulting from the inhalation of hazardous chemicals. To do so we obtained 20 individual realizations of a notional plume simulated by the VTHREAT modelling system, numerically estimated the ensemble mean plume from these realizations, and then compared the areas exceeding particular toxic load thresholds obtained from this ensemble mean plume to the areas derived from applying toxic load modelling to individual plume realizations.

The original toxic load model was derived from and experimentally fitted to population response data obtained from exposures of animals to a steady concentration of a toxic chemical in a closed chamber. To the best of our knowledge there is no official (or experimentally validated) extension of the toxic load model to time-varying concentration fields. Thus, we considered a total of four proposed extensions of the toxic load model to time-varying concentrations. We call these the Average Concentration, Integrated Concentration, Concentration Intensity, and Peak Concentration toxic load models.

Our comparison metrics include the "area above threshold" for a set of notional toxic load values and the ratio of this area calculated using an individual plume realization to the area calculated using the ensemble average of plume realizations.

Our main conclusion is that great care should be exercised when toxic load modelling is used to calculate the human health consequences of a toxic release. Most AT&D models that are presently used for consequence assessment predict ensemble mean plumes, which tend to be smoother in both space and time than the turbulent plumes that may be observed in a real event. Toxic load modelling magnifies the effects of localized (both in space and time) concentration "hot zones" for chemicals that have a toxic load exponent greater than 1, resulting in hazard areas derived from ensemble mean plumes that are significantly smaller than those derived from typical plume realizations. At higher toxic load thresholds, for which the most severe effects (e.g., deaths) are expected, the ensemble mean plume could greatly under-predict hazard areas. As mentioned earlier, for an actual release of hazardous material into atmosphere, individual people would be expected to be exposed to concentration realizations similar to individual concentration realizations (including fluctuations) predicted by VTHREAT and not the ensemble averaged plume produced by the majority of AT&D models in use today.

Additionally, while not explicitly mentioned in this paper, different toxic load models could produce very different estimates of the toxic load exposure given the same concentration profile and, as a result, produce very different estimates of hazard areas. There is no experimental evidence to either validate or refute different extensions of the toxic load model extensions that account for time-varying concentrations, but there are many such extensions being advocated for consequence assessment or even being used for that purpose. Thus, there is a great need to institute a research program to try to establish the validity of the toxic load models that have been proposed or are being used.

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REFERENCES

Bieberbach, G., Bieringer, P.E., Wyszogrodzki, A., Weil, J., Cabell, R., Hurst, J., and J. Hannan, 2010: Virtual chemical and biological (CB) agent data set generation to support the evaluation of CB contamination avoidance systems, The Fifth Symposium on Computational Wind Engineering (CWE 2010), Chapel Hill, North Carolina.

Sommerville, D.R., Park, K.Y., Kierzewski, M.O., Dunkel, M.D., Hutton, M.I. and N.A. Pinto, 2006: Toxic Load Modeling, in Inhalation Toxicology, Second Edition, edited by H. Salem and S.A. Katz, Boca Raton, FL, CRC Press, pp. 137-158.

Sommerville, D.R., Bray, J.J., Jablonski, R.E., Reutter-Christy, S.A. and E.E. Shelly, 2009: Review of Human Lethality Estimates for Chlorine Inhalation, Presentation J14.4 at the Eighth Symposium on the Urban Environment, 89th Annual American Meteorological Society Meeting, Phoenix, Arizona, January 2009

Stage, S.A., 2004: Determination of Acute Exposure Guideline Levels in a Dispersion Model, Journal of the Air & Waste Management Association, 54, pp. 49–59.

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

ten Berge, W.F., and M.V. van Heemst, 1983: Validity and accuracy of a commonly used toxicity-assessment model in risk analysis, Fourth International Symposium on Loss Prevention and Safety Promotion in Process Industries, Vol. 1, Institute of Chemical Engineers, Rugby, United Kingdom, pp. 11-112.

ten Berge, W.F., Zwart, A., and L.M. Appleman, 1986: Concentration-Time Mortality Response Relationship of Irritant and Systematically Acting Vapors and Gases, Journal of Hazardous Materials 13, pp. 301-309

Czech, C., Nathan Platt, Jeffry Urban, Paul Bieringer, George Bieberbach, Andrzej Wyszogrodzki and Jeffrey Weil, 2011: A comparison of hazard area predictions based on the ensemble-mean plume versus individual plume realizations using different toxic load models, Paper 2.5 at the Special Symposium on Applications of Air Pollution Meteorology, 91st Annual American Meteorological Society Meeting, Seattle, Washington, January 2011

Urban, J.T., Platt, N., Adelizzi, E.A., Bucher, C.R., Henrikson, J.T., and K. Papadantonakis, 2010: Evaluation of Transport and Dispersion Modeling Tools for Chemical Facilities Terrorism Risk Assessment Applications: Final Report, Institute for Defense Analyses Paper P-4605, prepared for the Chemical Security Analysis Center, U.S. Department of Homeland Security.