COMPARISON OF HAZARD AREA AND CASUALTY PREDICTIONS OF A SMALL-SCALE CHEMICAL ATTACK USING VARIOUS TOXIC LOAD TOXICITY MODELS

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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 Haber's Law, in which toxic effects depend only on the total inhaled dose. For many chemicals, however, it has been observed that duration of the exposure do matter and a generalized "toxic load" model better accounts for this duration dependence. However, the toxicity experiments that support the toxic load model used exposures to steady concentrations of toxic chemicals, whereas actual atmospheric chemical concentrations fluctuate in time over the exposure duration. In this study, we assess four proposed extensions of the toxic load model to the case of non-steady exposures that cover the full spectrum of conservatism in casualty and hazard area estimation. We used predictions of the turbulent toxic plume generated by the US National Center for Atmospheric Research (NCAR) Virtual Threat Response Emulation Test Bed (VTHREAT) high-performance computational modelling system to investigate how estimates the number of casualties and size of the hazardous area resulting from a small-scale chemical artillery attack vary among the four proposed toxic load models. Additionally, by rescaling the mass of the individual source terms (artillery shell impacts) and considering each source term individually, we investigated the sensitivity of the comparisons to source intensity changes that might be notionally applicable to a small-scale chlorine attack. We found that for a single realization of the small-scale chemical artillery attack, casualties and hazard areas predicted by different toxic load models sometimes differed from each other by almost a factor of two. However, when considering the individual chemical sources to represent different realizations of a chlorine release from a catastrophically-ruptured container, the hazard areas predicted by different toxic load models could differ by up to a factor of six. We conclude that the choice of the toxic load model used in hazardous materials consequence assessments can be important in the case of realistic time-varying toxic exposures.

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

INTRODUCTION

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. 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. The toxic load model of toxicity tries to account for this effect by applying an exponent to the concentration of inhaled chemical. Although the experimental data supporting the toxic load model were derived using rectangular-pulse concentration exposure profiles, actual atmospheric exposures resulting 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 toxicity 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 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 and AT&D modelling (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. Our earlier study (Czech et al., 2011) used 20 VTHREAT plume realizations of a 10-minute continuous release of a neutrally-buoyant tracer gas to examine the difference between using an ensemble-averaged plume to estimate casualties and the size of hazardous areas and using individual plume realizations. Since a short continuous release may not be fully representative of the conditions of a military attack using chemical weapons, our present study considers the same problem in the context of a small-scale chemical artillery attack.

For this study, VTHREAT was used to simulate 18 sources of a neutrally-buoyant gas, released instantaneously within a 200 meter by 100 meter zone. Since the gas is considered to be perfectly neutrally buoyant, the actual mass of each source does not affect the subsequent transport and dispersion of the gas, opening the possibility of interpreting the simulations in different ways depending on how much mass is associated with each source. For example, if each individual source represents about 1 kg of chemical agent, and the releases occur nearly simultaneously, the sources could be considered collectively to represent the impact of a salvo of chemical artillery rounds within a target box, as depicted in Figure 1. In this scenario, which was the principal subject of our study, a single VTHREAT simulation represents a *single realization* of a small-scale chemical artillery

attack. If, however, each individual source is considered to represent a quantity of agent on the order of hundreds to thousands of kilograms, then each source could be considered individually to represent the instantaneous release of a toxic industrial chemical (TIC) from a catastrophically-ruptured storage vessel. In this case, the VTHREAT simulation could be considered to represent multiple realizations of a TIC releases, albeit with the strong qualifier that the realizations are not truly independent since the dispersion from each simulated source will have some spatial and temporal correlations with the dispersion from nearby sources. Also, real TIC releases also often involve dense gas effects since a TIC is denser than air when released, either because of its high concentration and a molecular weight that is greater than that of air, or because it is cold due to refrigerated storage or autorefrigeration upon release. The VTHREAT simulations in this study do not account for dense gas effects. In this study, the scenario wind speed was set to 10 km/hr. Two sets of simulations were performed to produce one realization of the chemical attack for neutral atmospheric conditions and one realization for unstable (convective) atmospheric conditions.

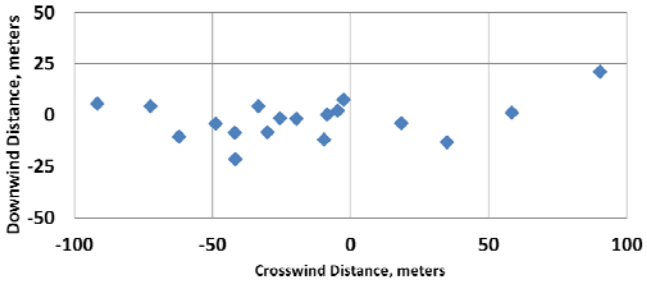

Fig.1: Location of 18 individual source terms used to simulate a small-scale chemical attack.

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:

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

where $D(\mathbf{x})$ denotes the dosage at a location $\mathbf{x}$ and $C(\mathbf{x})$ is a constant concentration to which a subject located at point $\mathbf{x}$ is exposed over a duration T. 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 $c(\mathbf{x},t)$ is quite prevalent (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 effects of such an exposure. 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 in 50% of the population.

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 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:

$$TL(\mathbf{x}) = C^n(\mathbf{x})T \tag{3}$$

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.

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 the case of non-steady exposures. Several such extensions have been proposed, but none have been validated experimentally.

In this paper we consider four different extensions of the toxic load model (TLM) to the case of time-varying concentrations: Average Concentration TLM (Hilderman et al., 1999), Integrated Concentration (or ten Berge) 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 Czech et al., 2011.

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

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

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

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

Here, $c(\mathbf{x},t)$ denotes concentration at spatial location $\mathbf{x}$ and time t, T denotes actual plume duration, c_{Peak} denotes the maximum concentration experienced at a given location $\mathbf{x}$, 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 inhaled dose only. It should be noted that for three of the toxic load models (Integrated Concentration, Concentration Intensity, and Peak Concentration) considered here it may be necessary to evaluate the toxic load using a concentration $c(\mathbf{x},t)$ that is time-averaged over some suitable time interval τ based on the effects of biological phenomena such as respiration and tissue uptake. It has been argued that the respiration rate places a lower bound on the value of τ, but its actual value – which may depend on the nature of the toxic substance, is generally unknown, so we introduce it as a parameter in our analysis.

BRIEF SUMMARY OF RESULTS: CASUALTIES AND HAZARD AREA COMPARISONS FOR A SINGLE REALIZATION OF A SMALL-SCALE CHEMICAL ARTILLERY ATTACK

Consider the VTHREAT simulation to represent a single realization of a small-scale chemical attack resulting from an artillery salvo that delivers 18 individual shells, each filled with 1.6 kg of the chemical warfare agent sarin, whose toxic load exponent is 1.5. Assuming that the population density is uniform, Fig. 2 shows the ratio of the number of casualties predicted by various toxic load models to the number of casualties predicted by the Integrated Concentration toxic load model for different concentration averaging time steps τ ranging from 1 second to 1 minute. We chose the Integrated Concentration toxic load model as the reference model because it appears to be the most commonly used extension of the toxic load model to the case for non-steady concentrations. As expected, as the concentration integration time step increases these ratios get closer to unity, since for large τ the concentration profile approaches that of a steady exposure, for which all time-dependent extensions of the toxic load model are expected to agree. For shorter concentration averaging times where there is less agreement between toxic load models, such as at τ = 5 seconds, the maximum casualty ratio among toxic load models is between the Peak Concentration and Average Concentration models, approximately 1.6.

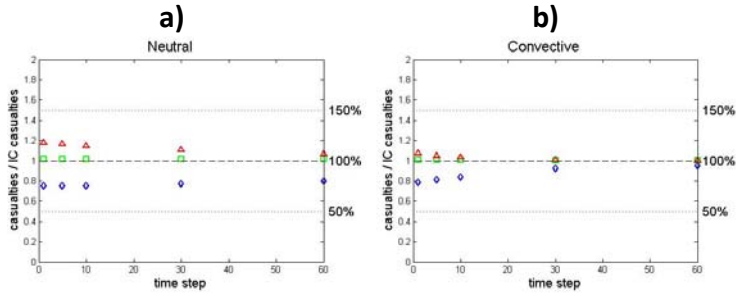

Fig.2: Ratio of the number of casualties as a function of the concentration integration time step. Panels a) and b) correspond to neutral and convective atmospheric conditions, respectively. The various toxic load models whose results are compared to the Integrated Concentration toxic load model are the Peak Concentration model (brown triangles), Concentration Intensity model (green squares), and the Average Concentration model (blue diamonds).

We also used the size of hazardous areas as a measure of consequences. We define the "hazard area" as the area over which a given threshold level of effects is exceeded. For sarin, we chose a variety of critical thresholds varying between 1% lethality and 99% lethality. The maximum ratio of the hazard area predicted by various toxic load models to the hazard area predicted by the Integrated Concentration toxic load model is approximately 1.7. Overall, for this particular *single realization* of a VTHREAT-simulated small-scale chemical attack under neutral and convective atmospheric conditions, we conclude that the difference between consequence estimates produced by different toxic load models can be up to a factor of two.

BRIEF SUMMARY OF RESULTS: HAZARD AREA COMPARISONS FOR MULTIPLE REALIZATIONS OF A CHLORINE RELEASE

Examining only a single realization of a sarin artillery attack presents some limitations in terms of conducting a robust examination of the effects of the choice of toxic load model on consequence assessment. First, one may be interested in specifically examining how the results change between realizations of a release. Furthermore, due to the relatively large probit slope associated with sarin, the dynamic range of relevant lethal exposure levels is rather narrow, spanning toxic loads from 93 to 230 $mg^{1.5}$-$m^{-3\times1.5}$-min. Consequently, only a relatively narrow portion of the sarin plume dominates the consequence estimates, and it is possible that the results for the small-scale sarin attack cannot be generalized to larger or smaller attacks or to the release of an agent with appreciably different toxicity parameters.

If we consider the 16 individual source terms in our chemical attack scenario to be multiple realizations of the same release and rescale the mass of each release significantly upward, then each of the 18 instantaneous source terms simulated in VTHREAT could be considered representing a catastrophic rupture of an industrial chemical storage vessel. Specifically, we considered the release of chlorine from two 150 lb cylinders (total release size = 136 kg) or from 1 US ton (908 kg) or 10 US ton (9080 kg) storage vessels. Chlorine has a lower probit slope than sarin, but a higher Eff_{50} for lethal effects and a higher toxic load exponent. We note that we did not account for the dense-gas effects that are normally associated with industrial chlorine releases and that these 18 releases are not entirely statistically independent of each other due to correlations in turbulence between closely-spaced sources. We also note that all four of the toxic load models described in Eq. 4-7 are amenable to a rescaling of the toxic load when concentration is rescaled:

$$TL(\alpha c(\mathbf{x})) = \alpha^n TL(c(\mathbf{x})) \tag{8}$$

This scaling relationship can be used to "normalize" toxic loads according to release mass. Fig. 3 depicts the ratio of the hazard area predicted by various toxic load models to the hazard area predicted by the Integrated Concentration toxic load model as a function of the toxic load threshold (averaging time τ = 5 seconds). A range of toxic loads is experienced within different parts of the hazardous plume for different release masses, since (for example) a 10% probability of lethality is possible much farther from the release source for a large release than for a small one. As can be seen from this figure, there is a considerable variation in the size of the hazardous area predicted by different toxic load models. There is also considerable variation in the size of the hazardous area among individual realizations of the release and among different release masses. In order to gain a quick appreciation for the size of these variations, consider the largest ratio of hazard areas between the Peak Concentration and Average Concentration toxic load models observed either among individual realizations of the release, or for the ensemble-average hazard area (i.e., the average over the 18 individual hazard areas) for the three release sizes mentioned above. Table 1 identifies the maximum ratio for toxic load thresholds only within the 1% to 99% lethality range for a given release size (i.e., the regions of Fig. 3 in between the pairs of vertical bars). We note that for the scaled chlorine release scenario, hazard area calculations could differ by up to a factor of 6 among individual realizations of the chlorine attack depending on the choice of toxic load model, and up to a factor of 3.3 for the ensemble-averaged hazard area.

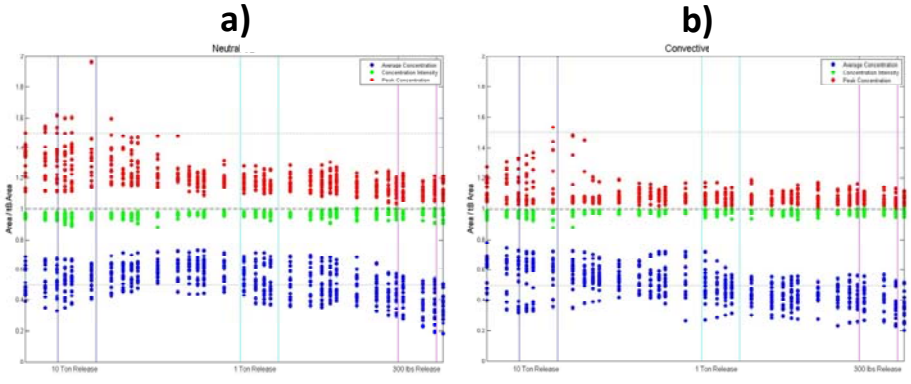

Fig.3: Ratio of the hazard area as a function of the toxic load threshold. Panel (a) shows results for neutral atmospheric conditions and panel (b) shows results for convective atmospheric conditions. The horizontal axis is on a logarithmic scale and has been rescaled into dimensionless units according to release mass. Pairs of vertical lines depict the span of toxic loads from 1% to 99% probability of lethality for different release masses. The various toxic load models whose results are compared to the Integrated Concentration model are the Peak Concentration model (red dots), Concentration Intensity model (green dots), and the Average Concentration model (blue dots). Individual dots represent individual chemical sources.

Table 1: Largest ratio of hazard areas between toxic load models for three release sizes for neutral and convective atmospheric conditions. The ratio maximums are calculated either among individual realizations of the release or for the ensemble-averaged hazard areas, for toxic loads in the 1% to 99% lethality range for a given release size.

	Neutral Atmosphere		Convective Atmosphere	
Release Mass, kg	Individual Realizations Max Ratio	Ensemble-Avergage Max Ratio	Individual Realizations Max Ratio	Ensemble-Avergage Max Ratio
136	4.2	2.3	3.8	2.1
908	3.1	2.3	4.3	2.3
9080	6.1	3.3	4.6	3.0

CONCLUSIONS

The VTHREAT modelling system was used to provide individual predictions of the neutrally-buoyant gas dispersion from 18 closely-spaced instantaneous chemical sources for neutral and convective atmospheric conditions with a 10 km/hr wind. When combined together, these 18 chemical sources could be thought of as notionally representing *single realization* of a small-scale chemical artillery attack. Taken individually, and scaled according to release mass (136 kg, 908 kg, and 9080 kg), these 18 source terms could notionally represent 18 individual (albeit correlated) realizations of a chlorine release from a catastrophically-ruptured container.

The original toxic load model was derived from toxicity experiments on animals exposed to a steady concentration of toxic chemical over a finite duration. To the best of our knowledge, there is no accepted or experimentally validated extension of the toxic load model to the case of time-varying exposures, which is the situation that is expected to be encountered in real-world incidents. We considered the difference between the predictions of toxic hazards between four proposed extensions of the toxic load model to the case of time-varying exposures. We examined either the ratio of casualties or the size of hazardous areas upon choosing one of the toxic load models as an arbitrary baseline.

For a single realization of the small-scale chemical artillery attack, casualties and hazard areas predicted by different toxic load models sometimes differed from each other by almost a factor of two. However, when considering the individual chemical sources to represent different realizations of a chlorine release from a catastrophically-ruptured container, the hazard areas predicted by different toxic load models could differ by up to a factor of 6. Moreover, the hazard area computed by averaging over all of the 18 individual releases still can differ among the various toxic load models by up to a factor of 3. We conclude that the choice of the toxic load model used in consequence assessments can be important in the case of realistic time-varying toxic exposures.

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