Institute for Defense Analyses
4850 Mark Center Drive • Alexandria, Virginia 22311-1882 • U.S.A.

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Comparison of hazard area and casualty predictions of a small-scale chemical attack using various toxic load toxicity models

Jeffry T. Urban, Keith Galvin, Nathan Platt

Institute for Defense Analyses

Paul Bieringer, George Bieberbach, Andrew Annunzio

US National Center for Atmospheric Research

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Introduction

- During the past 10 years, some workers in the hazardous materials consequence assessment modelling community have moved toward using “toxic load”-based models of acute inhalation toxicity
  - The toxic load is a generalized measure of inhalation exposure that depends on the time history of the exposure

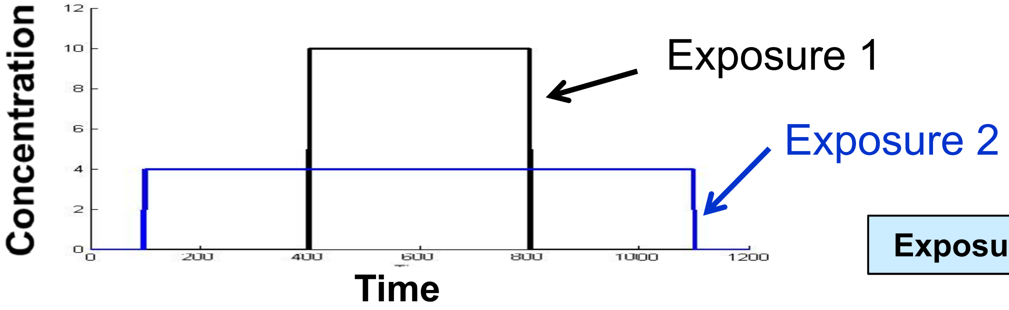
- This adoption of toxic load modelling has preceded a full understanding of its application to atmospheric dispersion modelling
  - Toxic load modelling has been experimentally validated only for steady-exposures – several models have been employed to account for fluctuating concentrations, but none have been validated
  - Most atmospheric dispersion models predict an ensemble-averaged plume that reduces the concentration fluctuations to which some toxic load models are sensitive

- In this work we model individual realizations of a small-scale chemical artillery attack to compare different proposed toxic load models
  - A subsequent presentation deals with the prospects of using SCIPUFF probabilistic plume information in place of ensemble-averaged plumes

Haber's Law and toxic load for steady exposures

- Haber's Law says that the probability of casualty depends only on the dosage, $D(r) = C(r)\,T$, for steady concentrations C(r) over time T (at location r)

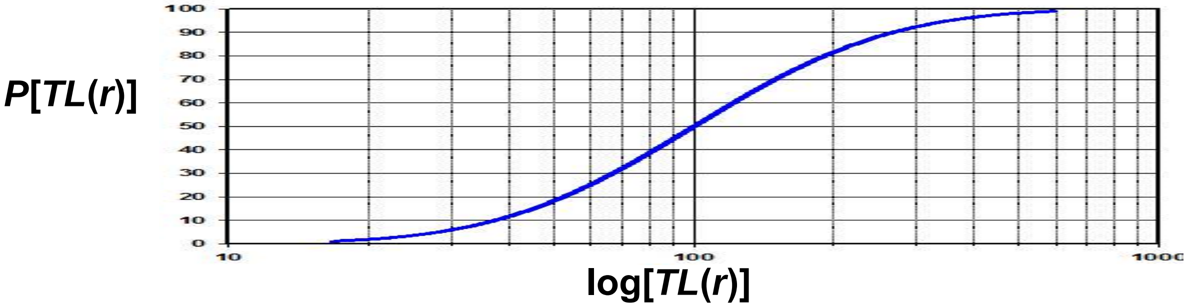
- For some toxic materials, the probability of casualty is better modeled by replacing the dosage with the "toxic load", $TL(r) = [C(r)]^n\,T$
    - Unlike Haber's law, the ratio of concentration intensity to duration matters
    - n is an extra toxicity parameter called the toxic load exponent ($n = 1$ → Haber's Law)



Two exposures:
<u>same</u> *dosage*,
<u>different</u> *toxic load*

Exposure 1 has the greater toxic load for *n* > 1.

- Toxic load/dosage are lognormally related to the probability of casualty:



Two toxicity parameters:

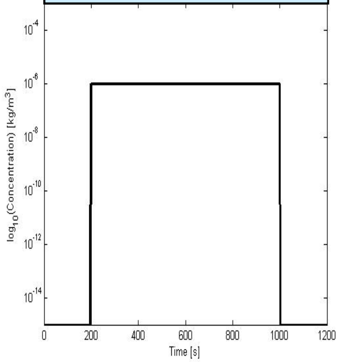
μ (log[median effective TL])

σ (reciprocal of "probit slope")

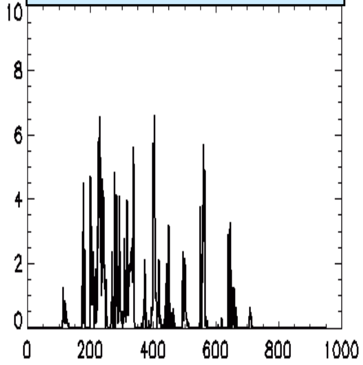
Time-Dependent Toxic Load Models

Several toxic load models have been proposed, *but not experimentally validated*, for the case of time-varying exposures

Laboratory Exposure



Possible Real-World Exposure



- ten Berge Model (integrate c***n*** over time)

$$TL_{TB}(x) = \int c^n(\tau)\,d\tau$$

- Average Concentration Model (use average C over exposure duration)

$$TL_{AC}(x) = \left(\frac{\int_{t_{start}}^{t_{end}} c(\tau)\,d\tau}{T} \right)^n T = D^n T^{1-n}$$

$$\boxed{D = \int c(\tau)\,d\tau}$$

- Peak Concentration Model (use maximum C over *effective* exposure duration)

$$TL_{PC}(x) = D^n T^{1-n} \text{ where } T = \frac{D}{C_{peak}}; TL(x) = \frac{D}{C_{peak}^{1-n}}$$

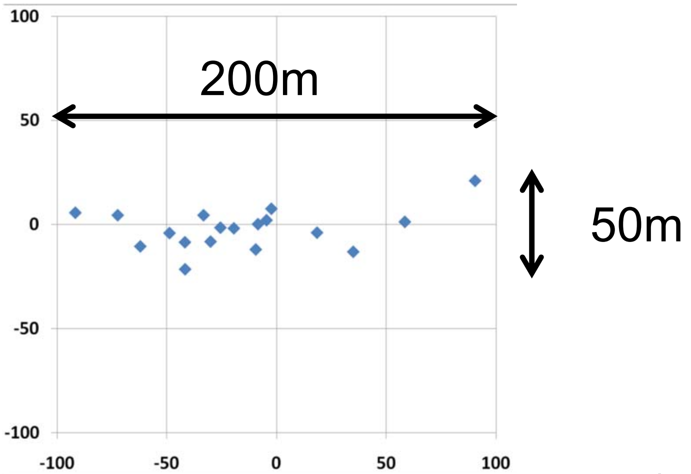
- Concentration Intensity Model (concentration variance effective exposure)

$$TL_{CI}(x) = D^n T^{1-n} \text{ where } T = \frac{\left(\int c(\tau)\,d\tau\right)^2}{\int c(\tau)^2\,d\tau} = \frac{D^2}{\int c(\tau)^2\,d\tau}; TL(x) = \frac{D^{2-n}}{\left(\int c(\tau)^2\,d\tau\right)^{1-n}}$$

Comparison of different toxic load models using simulations of a realistic chemical attack

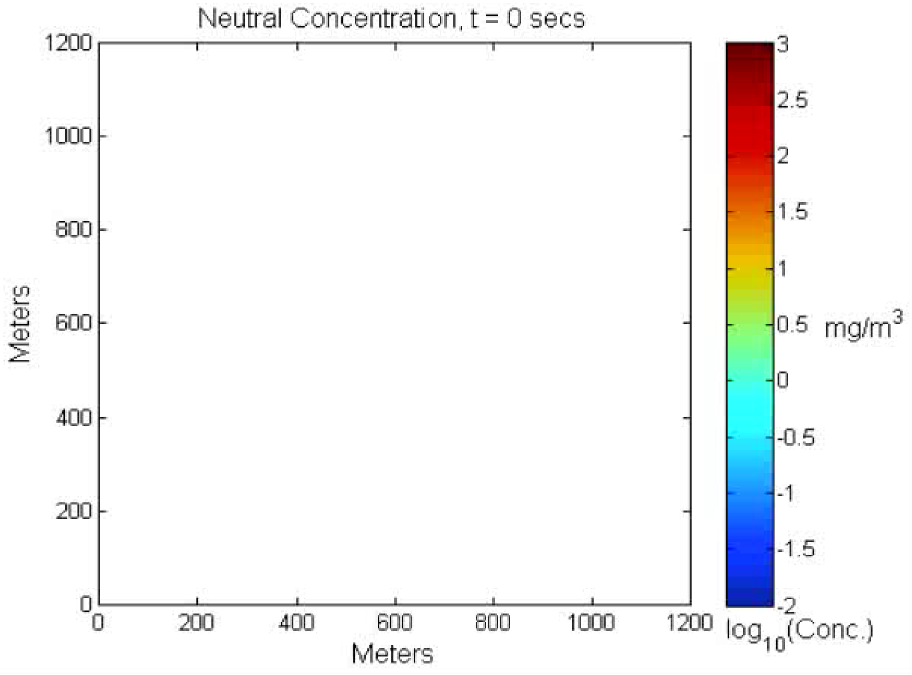
- Question: How much do consequence estimates differ among these four proposed toxic load models?

- We used NCAR’s VTHREAT simulation environment to produce four turbulent realizations of a small-scale chemical attack involving 18 artillery shells (152mm diameter) filled with Sarin nerve gas ($n = 1.5$)
  - 2 different atmospheric stability conditions (neutral and unstable (convective))
  - 2 different wind directions (parallel and perpendicular to 200m × 50m impact area)
- For each combination of atmospheric stability and wind direction compare:
  - Casualty Estimates
  - Hazard Area Predictions



VTHTREAT simulations of the Sarin attack

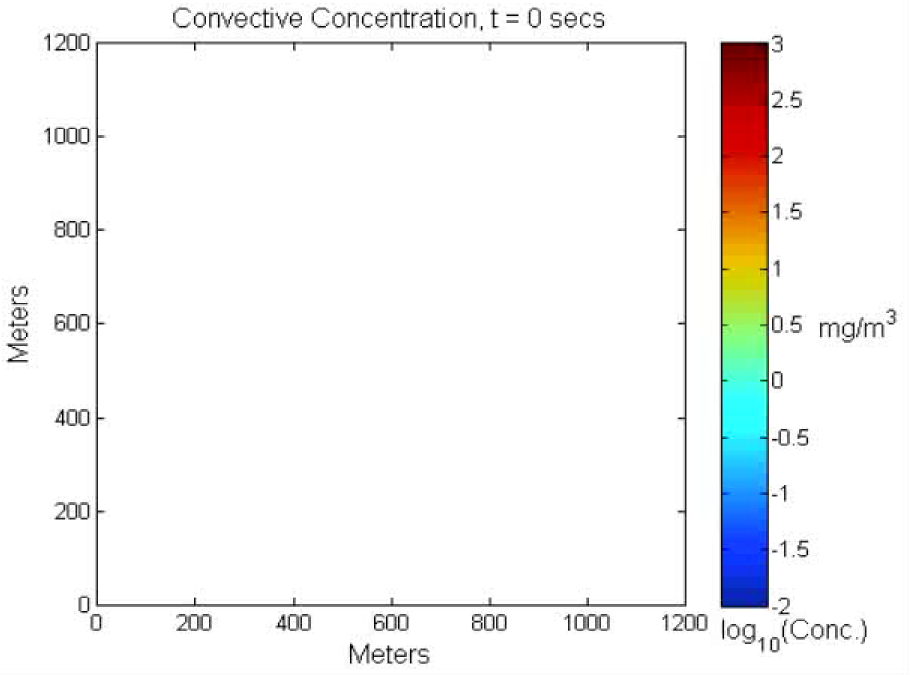
Neutral atmospheric conditions



Wind direction

→

Convective atmospheric conditions



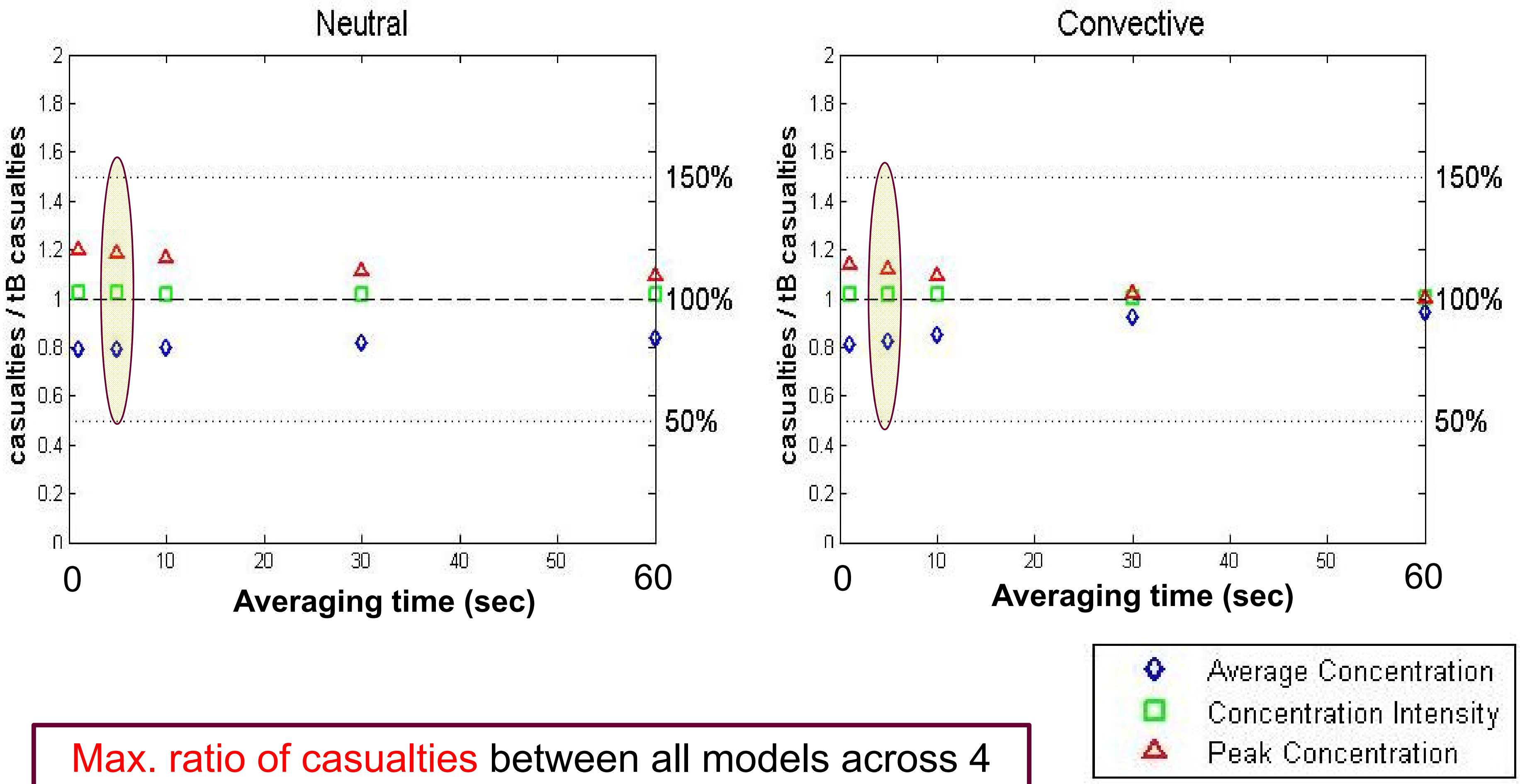
Wind direction

→

Toxic load model casualty estimates for Sarin

Ratio to ten Berge model casualties as a function of averaging time

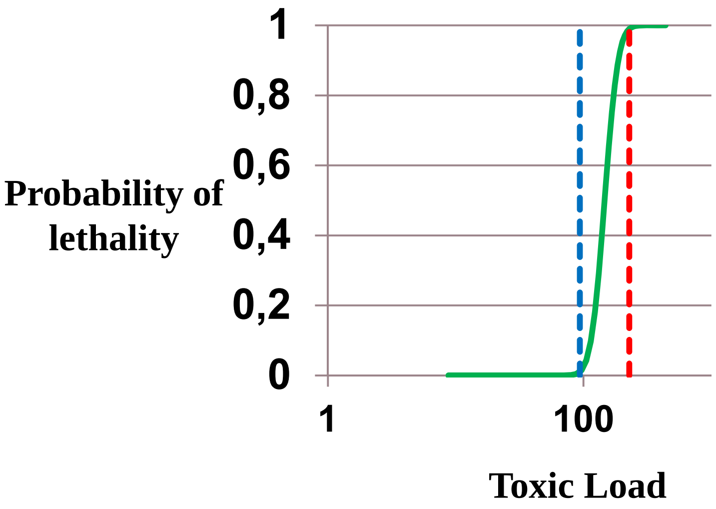
(Wind parallel to attack axis)



Max. ratio of casualties between all models across 4 VTHREAT simulations (5-sec time step) = 1.58

Sensitivity of results to the lethal range of toxic loads

- The VTHREAT predictions exhibit a wide dynamic range of toxic loads
  - TL range of [0, 33000]
- However, Sarin lethal effects are observed over only a small dynamic range of toxic loads (reflecting the large probit slope for Sarin)
  - TL range of [94, 229] corresponding to [1%, 99%] probability of lethality

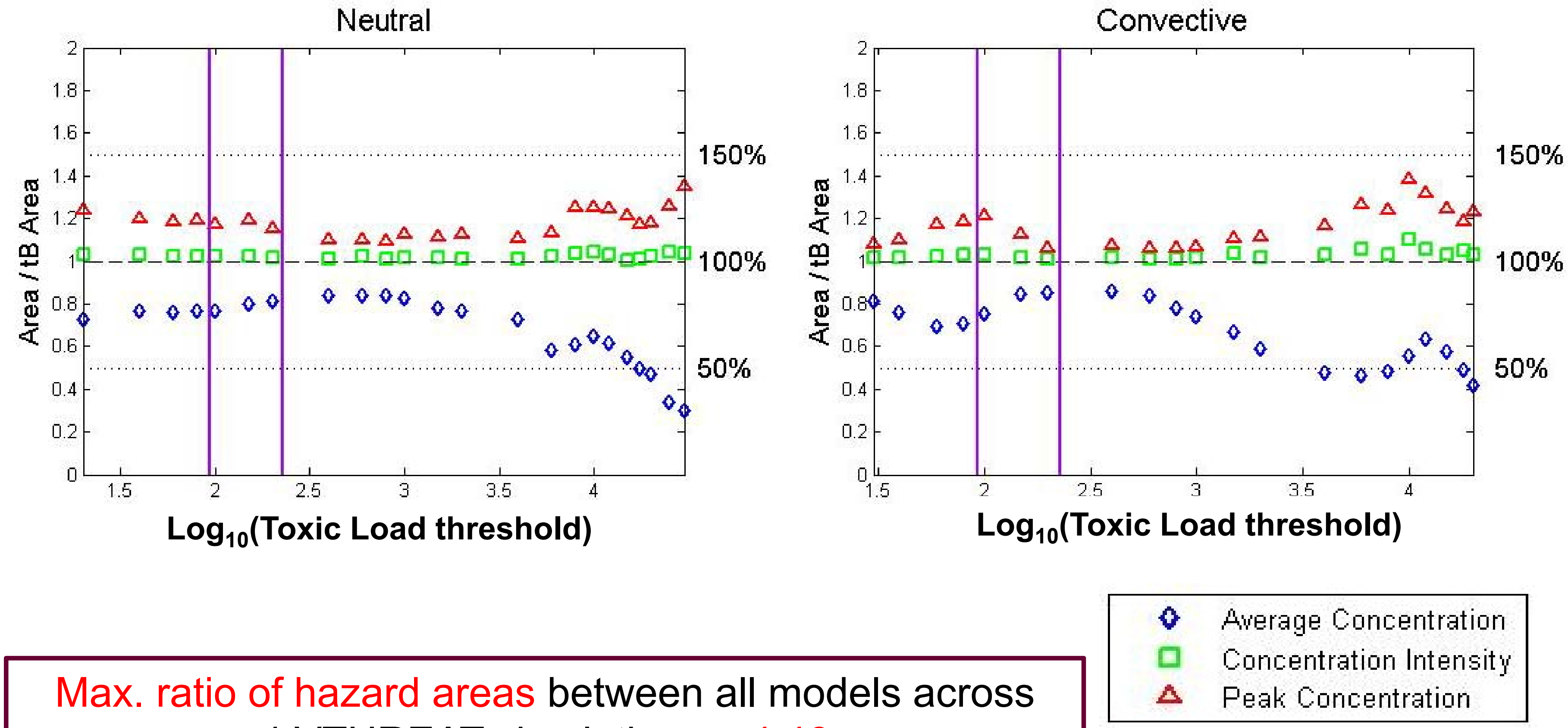


- Are our casualty results dependent on this choice of a narrow range of toxic loads of interest? We investigated this question by examining the areas of exceedance for different toxic load thresholds.

Toxic load model hazard area estimates for Sarin

Ratio to ten Berge model hazard area as a function of toxic load threshold

(Wind parallel to attack axis)



Max. ratio of hazard areas between all models across 4 VTHREAT simulations = 4.46
(greater difference between models at higher toxic loads)

Study Excursion – Chlorine Attack

- Question: How would choosing a different chemical with significantly different toxicity, or a different release mass, affect differences between consequence estimates among various toxic load models?

- We randomly chose one source out of the 18 sarin munitions to serve as a surrogate for an industrial chlorine container
  - VTHREAT can be used to represent any neutrally-buoyant release (ignoring the significant chlorine dense gas dispersion effects)

- Chlorine differs significantly from Sarin in terms of toxicity
  - $n = 2.75$ (vs. $n = 1.5$ for Sarin)
  - LD_{50} = 13,500 mg-min/m^3 for a two-minute exposure (vs. LD_{50} = 35 for Sarin)

- Examined 9080 kg (10 short tons), 908 (1 short ton), and 136 kg (two 150 lb cylinders) releases

- All of the toxic load models scale the same way w.r.t. release mass

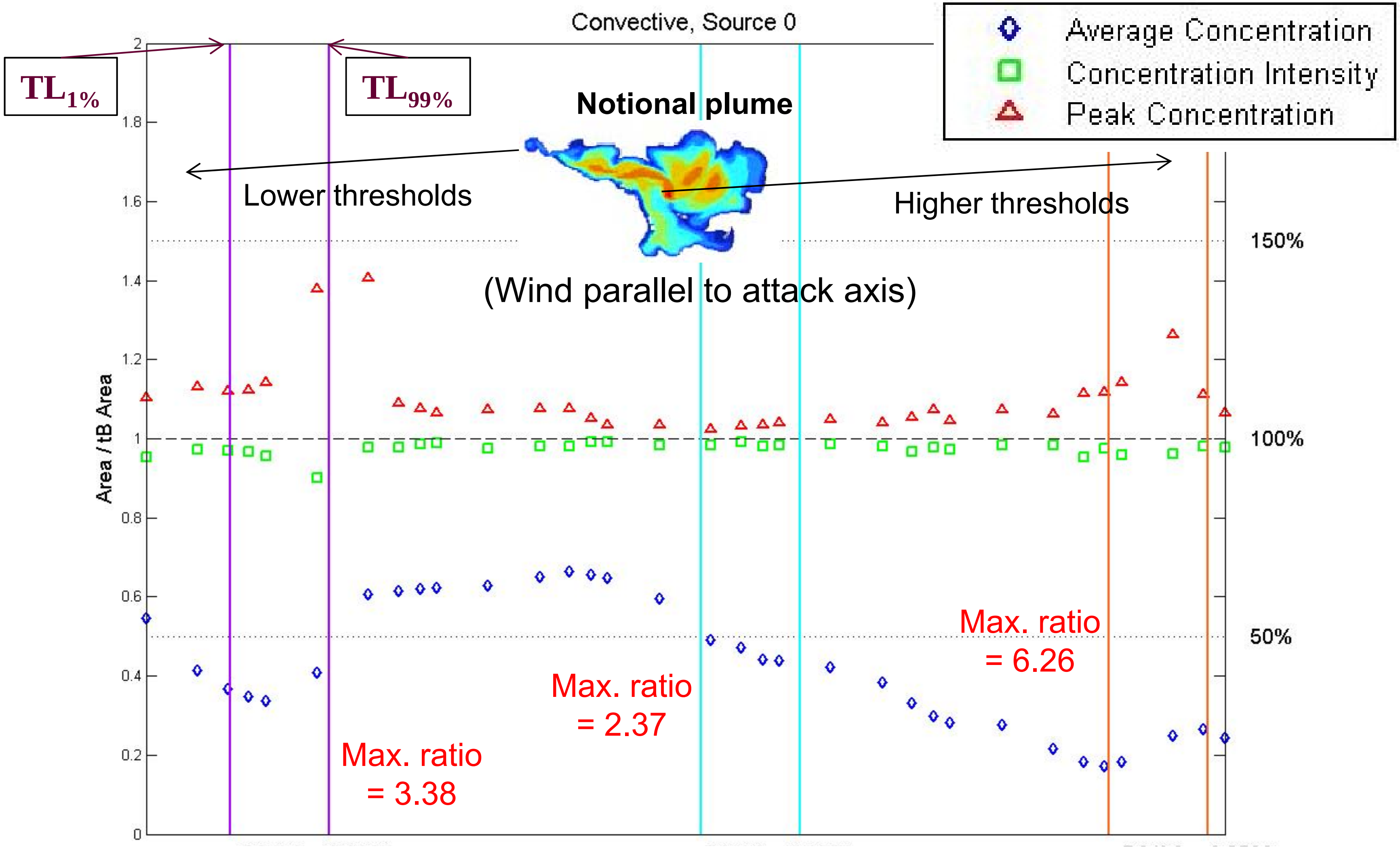
$$TL(\alpha x) = \alpha^n TL(x)$$

  - This scaling can be used to normalize "toxic load exposure" in terms of release mass for the plots on the next pages

Toxic load model hazard area estimates for Chlorine

Convective atmospheric conditions, single source

Ratio to ten Berge model hazard area as a function of toxic load threshold



(Wind parallel to attack axis)

Max. ratio = 3.38

Max. ratio = 2.37

Max. ratio = 6.26

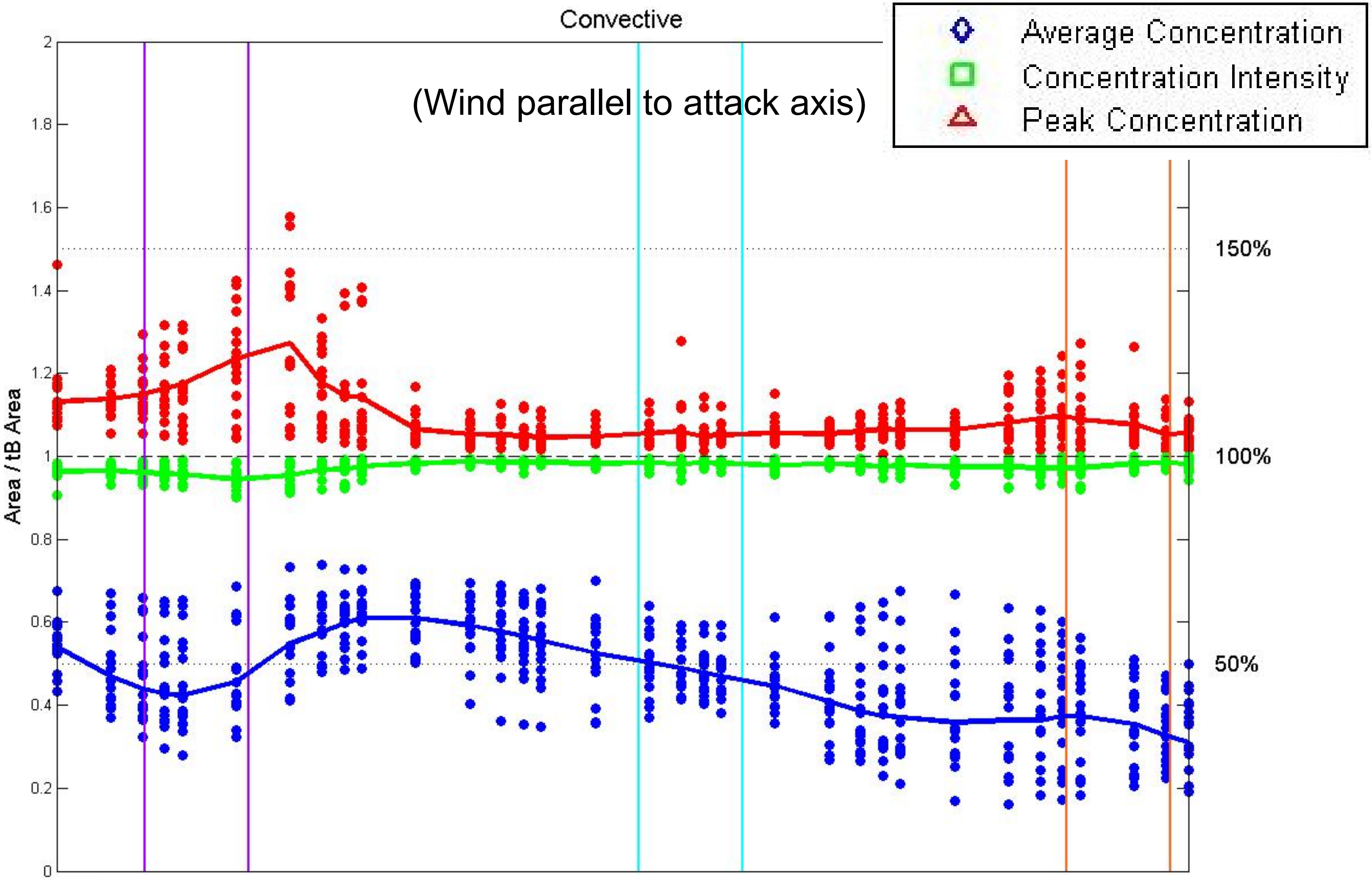
10 Ton release **1 Ton release** **136 kg release**

Toxic load threshold level (scaled to unit release mass)

Toxic load model hazard area estimates for Chlorine

Convective atmospheric conditions, <u>all 18 sources</u>

Ratio to ten Berge model hazard area as a function of toxic load threshold



10 Ton release **1 Ton release** **136 kg release**

Toxic load threshold level (scaled to unit release mass)

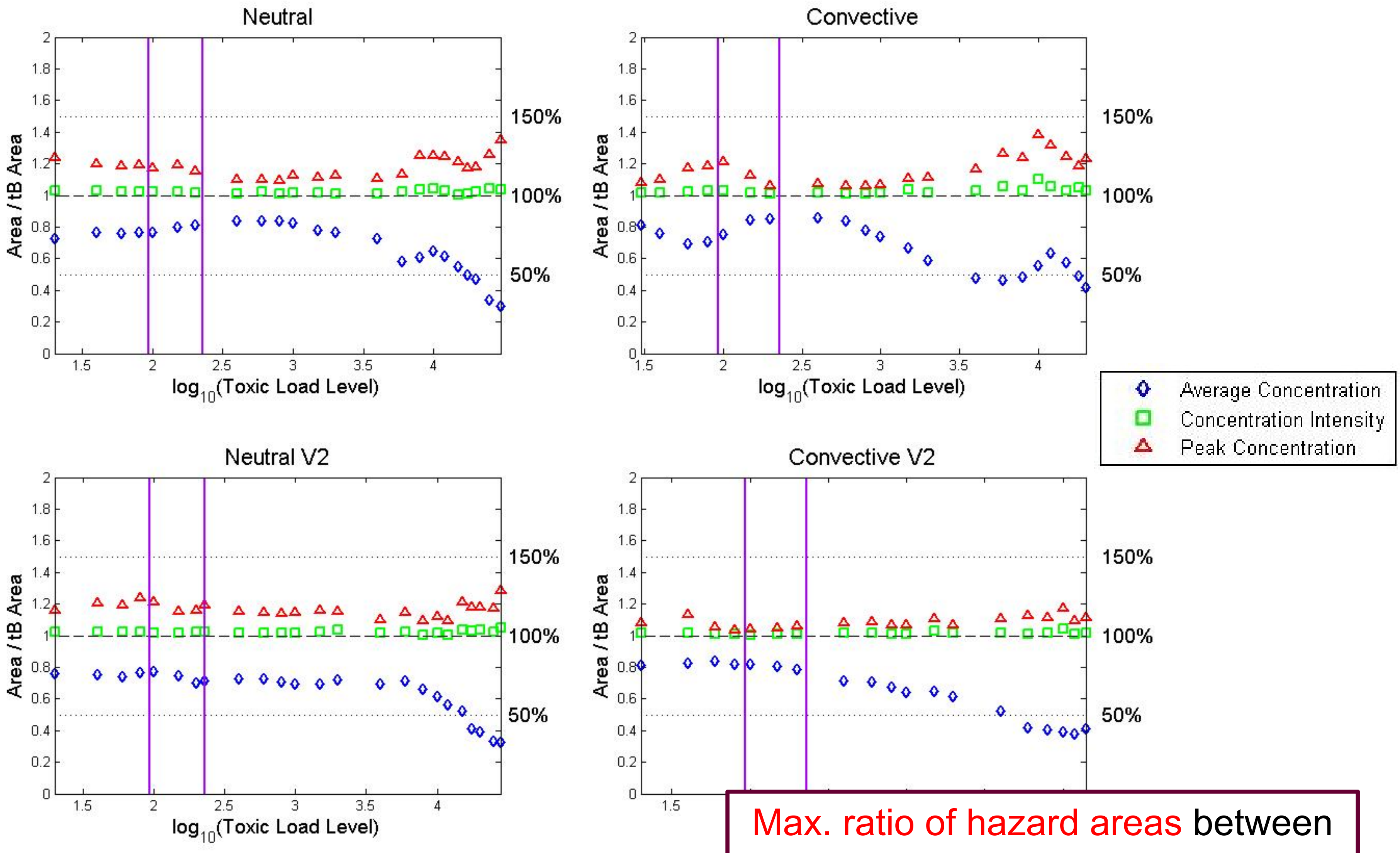
Conclusions

- We investigated the differences between four proposed time-dependent toxic load models using casualty and hazard area estimates based on simulations of a realistic chemical attack
- The differences between models were not large for an 18-shell Sarin artillery attack: up to a factor of ~1.5 in casualty estimates for a 5 s concentration averaging time
    - Differences were even smaller for longer averaging times
- For a notional industrial chlorine release (ignoring dense gas effects), the differences among models were larger (up to a factor of ~2-6)
- The peak concentration toxic load model gave the largest consequence estimates and the average concentration model gave the smallest
- Consequence estimates can differ considerably among the models according to the choice of chemical and size of release (and to a lesser extent, the averaging time)

Backups

Threshold Area Relative to “tB” Threshold Area

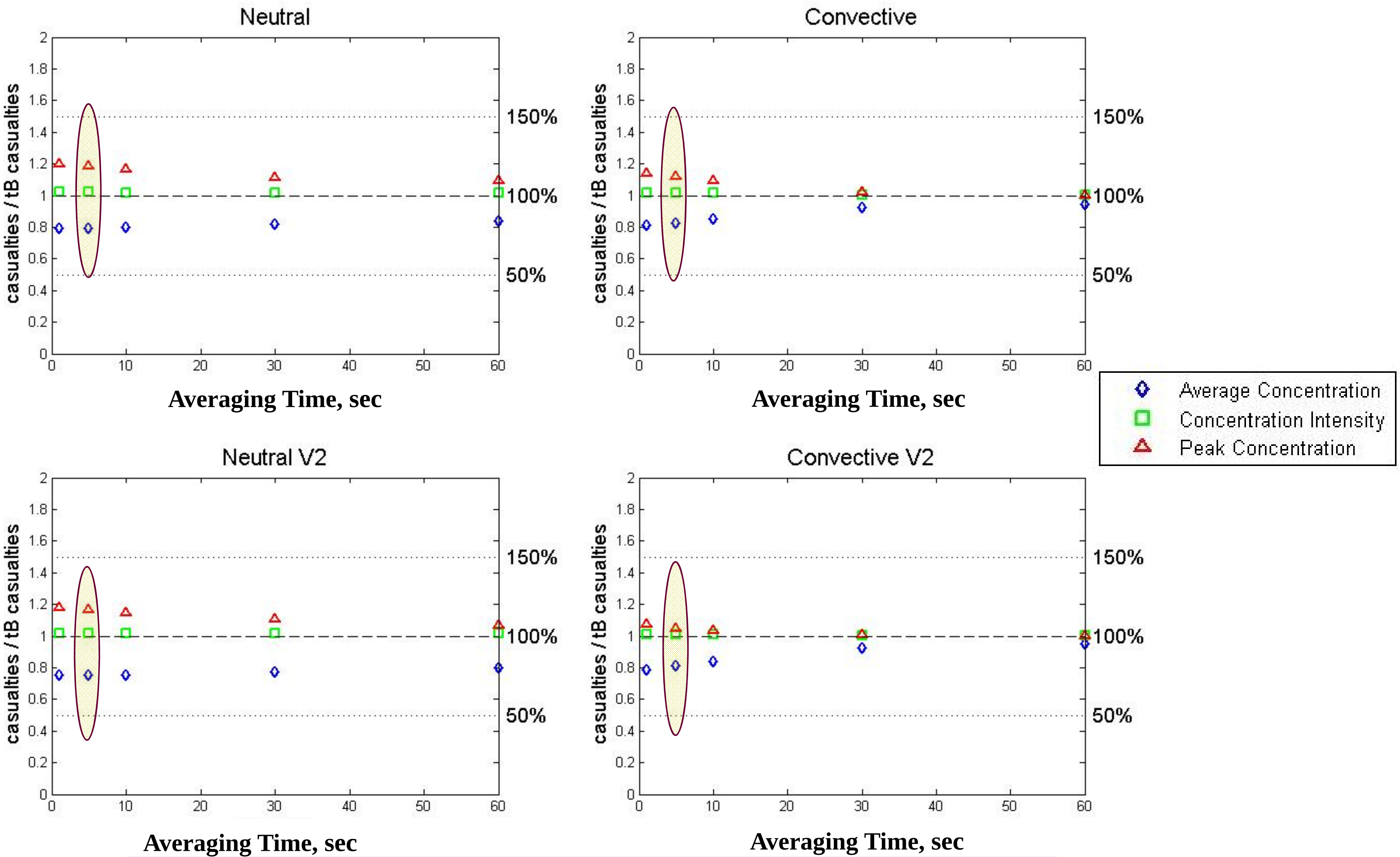
Full range of Toxic Load Exposure



Max. ratio of hazard areas between all models across 4 VTHREAT simulations = 4.46

Casualties Relative to ten Berge (tB) Casualties

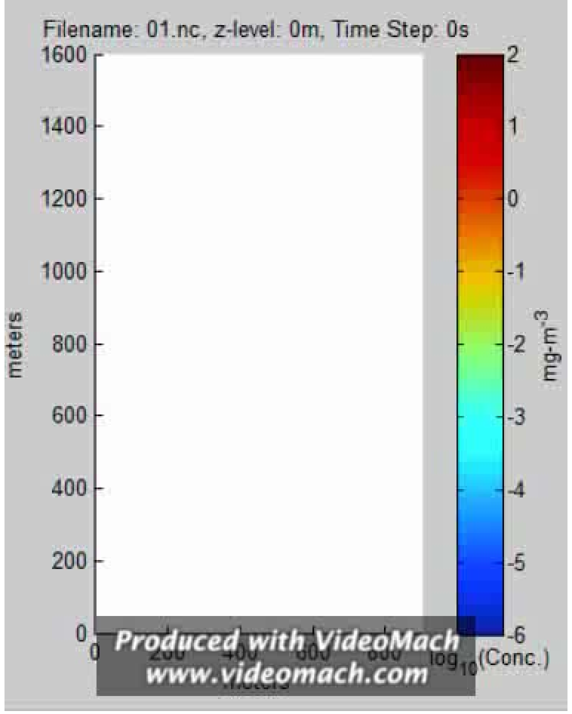
As a Function of Time Averaging



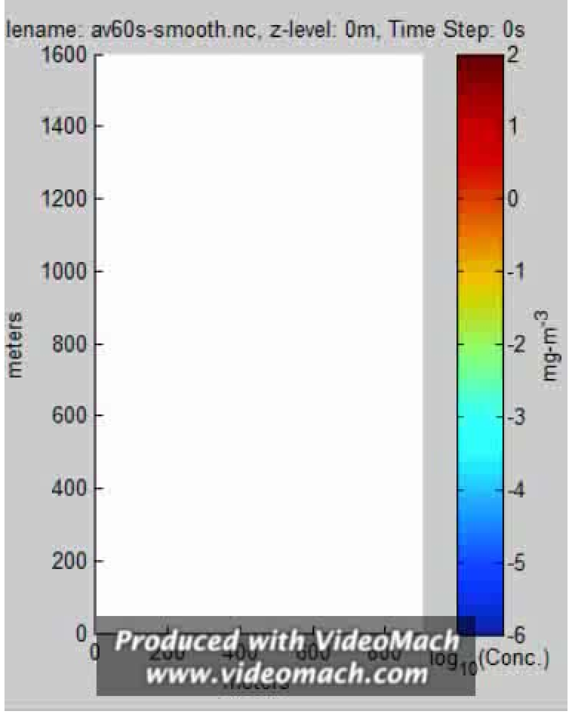
Max ratio between all models (5-sec time step) = 1.58

Ensemble-Average Plume Predictions

- Most AT&D models produce a “mean” plume that represents an ensemble average of many different turbulent realizations of individual plumes.
  - By definition, these mean plumes smooth out concentration fluctuations in time and space



Individual Plume Realization
One of twenty different realizations of
a simulated plume release.



Temporally Averaged Ensemble Average
Constructed from the limited ensemble average
with a 60-second running window average

The VTHREAT simulations used in to create above plumes represent relatively stable atmospheric conditions.

Haber's Law and Toxic Load Models

- Most AT&D models calculate toxic effects as a function of only the total dosage of the exposure (Haber's Law).
  - Haber's Law relationships are established empirically for dosages based on constant-concentration exposures:

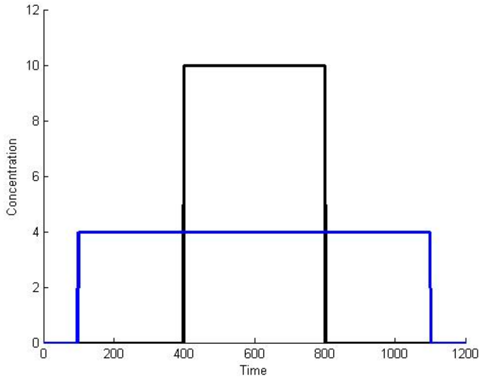
$$D(\mathbf{x}) = C(\mathbf{x})T$$

  - A (unproven) generalization of Haber's Law for time-dependent concentrations defines dosage as:

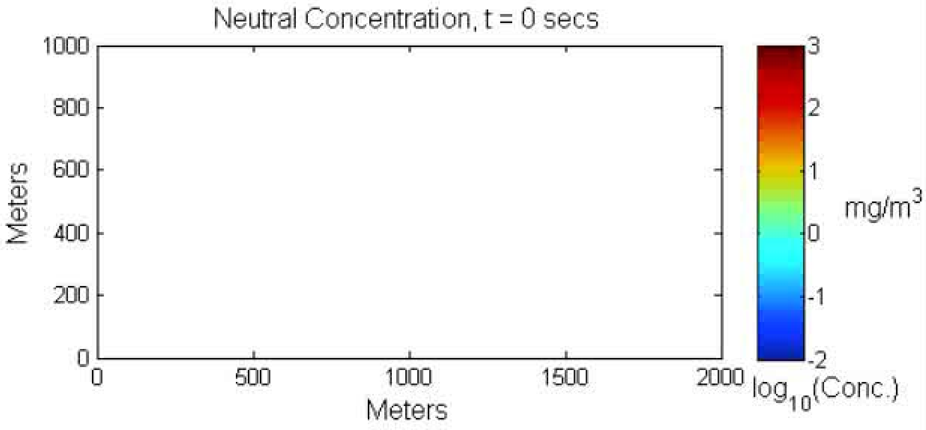
$$D(\mathbf{x}) = \int_{t_i}^{t_f} c(\mathbf{x},t)dt$$

  - Haber's Law implies that, assuming the same total dosage, both high-concentration short-duration exposures and low-concentration long-duration exposures result in the same toxic effect.
- Early experiments showed that Haber's Law does not hold for some chemicals.
  - The toxic effects of these chemicals are better described when the dosage is replaced by a generalized "Toxic Load"
  - For *n* > 1, high-concentration short-duration exposures will produce a stronger toxic effect than low-concentration long-duration exposures.

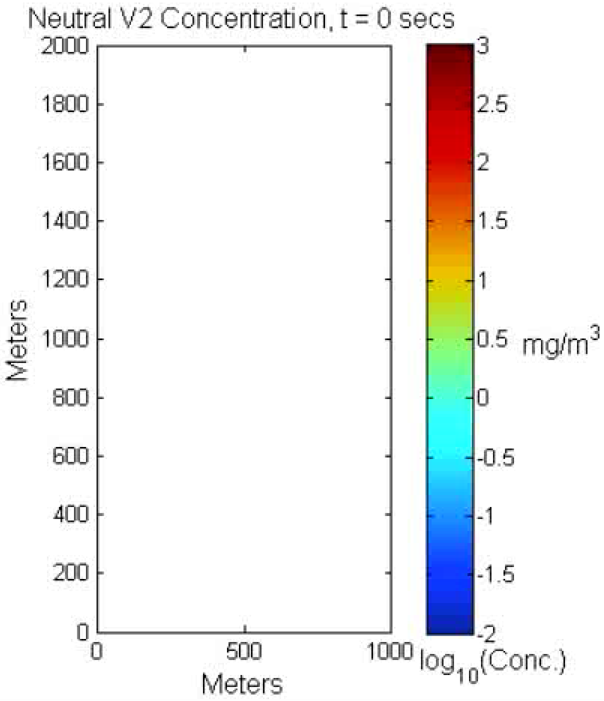
$$TL(\mathbf{x}) = (C(\mathbf{x}))^n T$$



Neutral Release – Individual Realizations



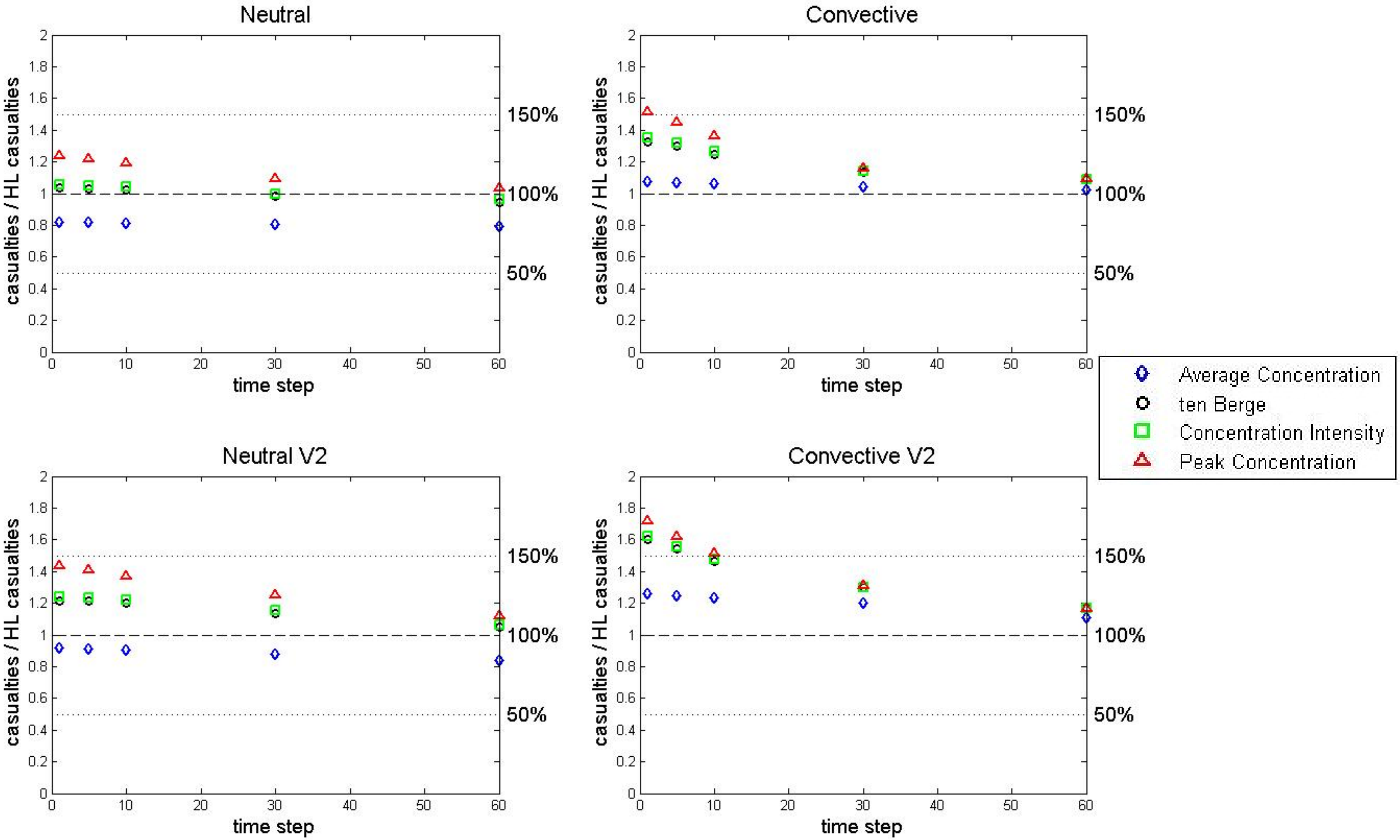
Wind parallel to long axis of impact pattern



Wind perpendicular to long axis of impact pattern

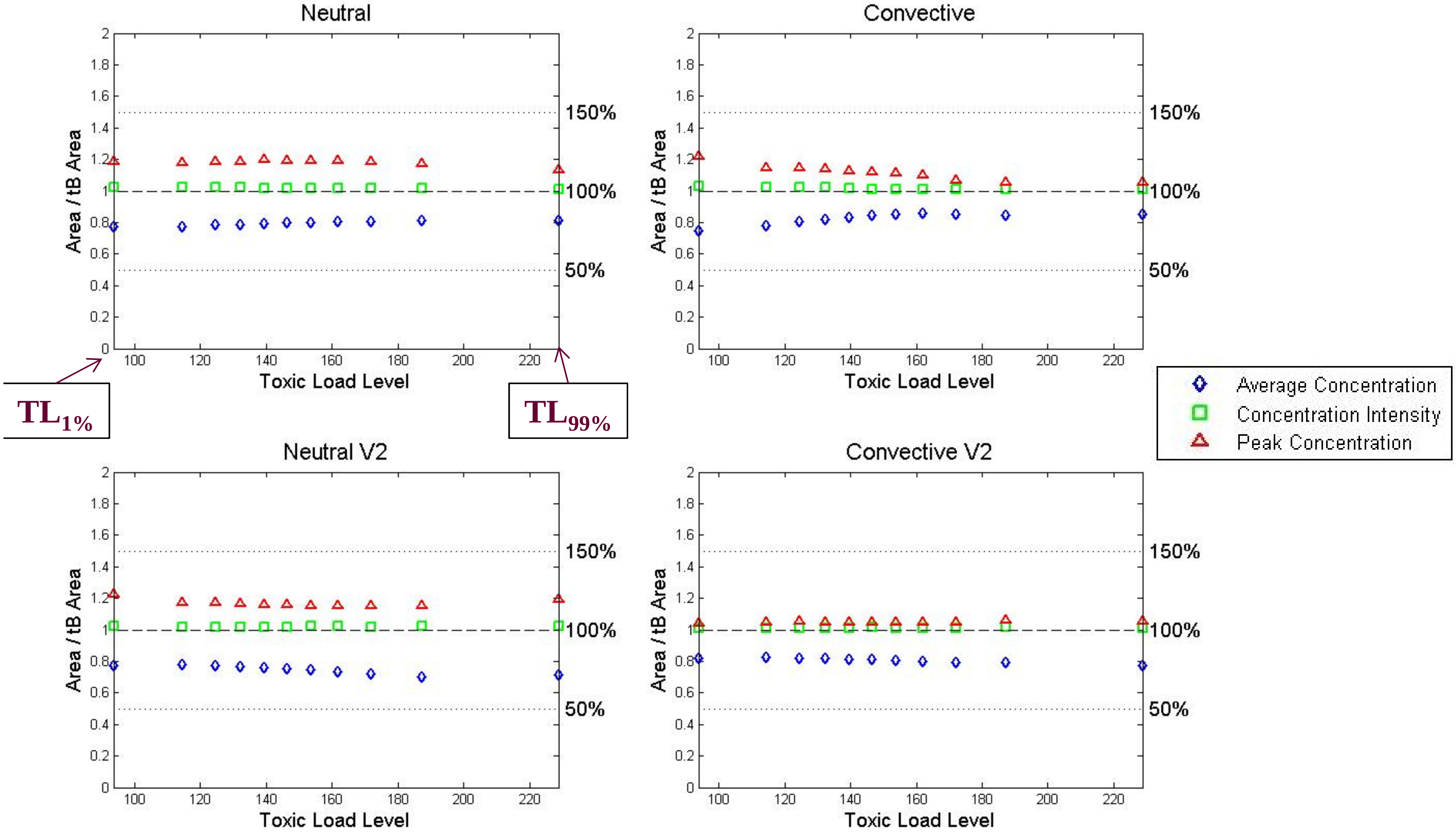
Casualties Relative to Haber’s Law (HL) Casualties

As a Function of Time Averaging



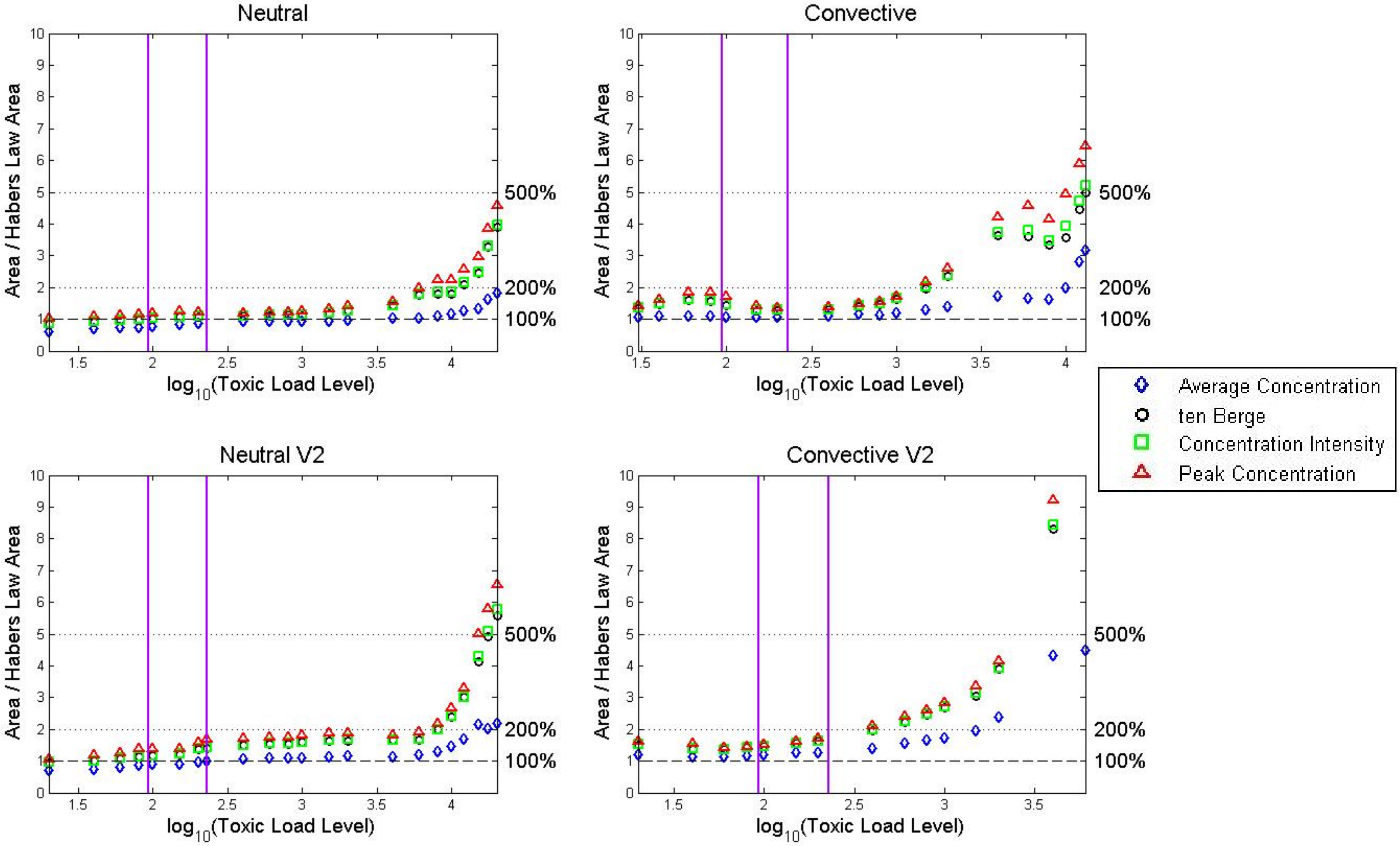
Max ratio between all models (5-sec time step) = 1.61

Threshold Area Relative to “tB” Threshold Area



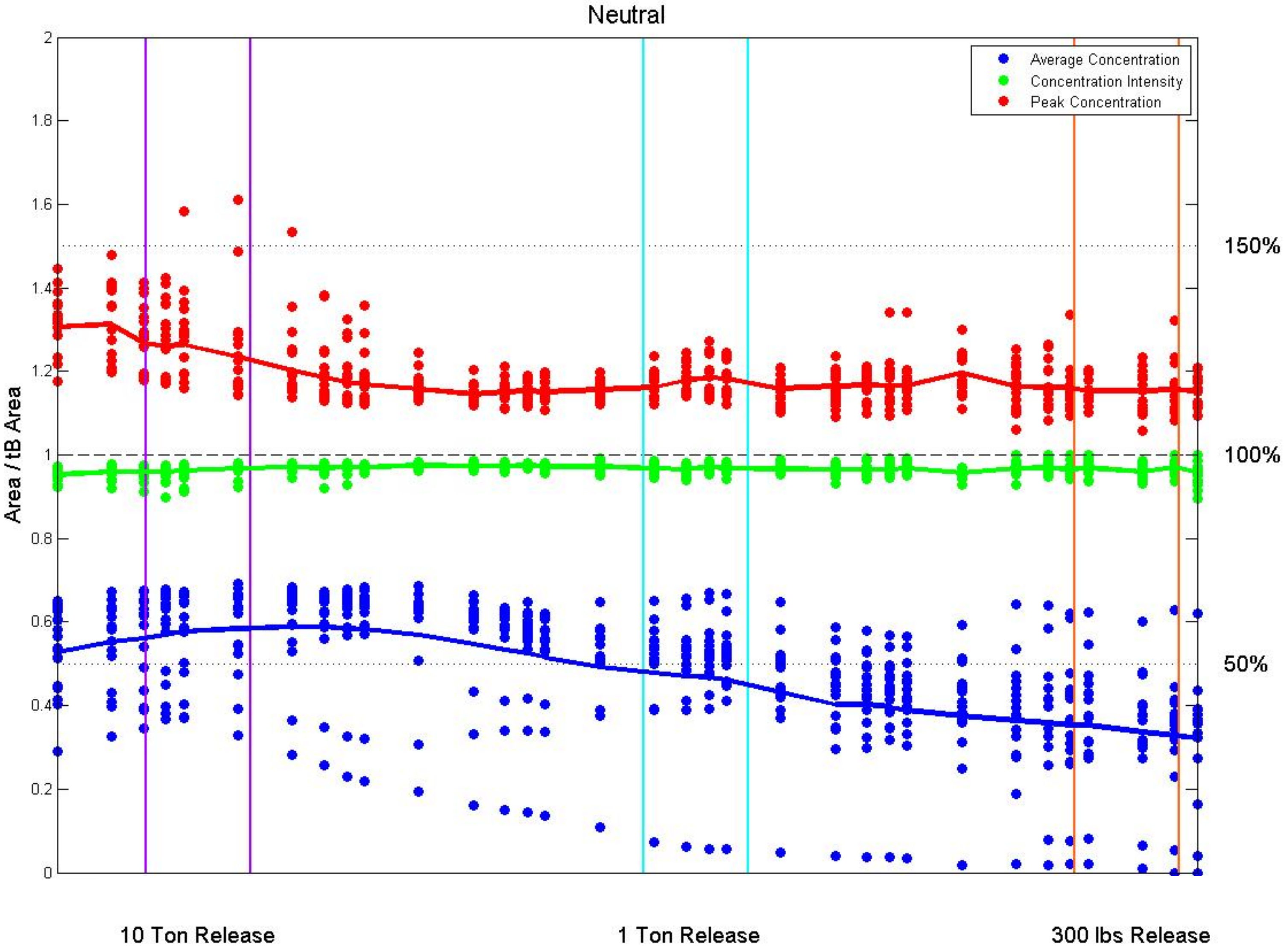
Max ratio between all models = 1.68

Threshold Area Relative to “HL” Threshold Area

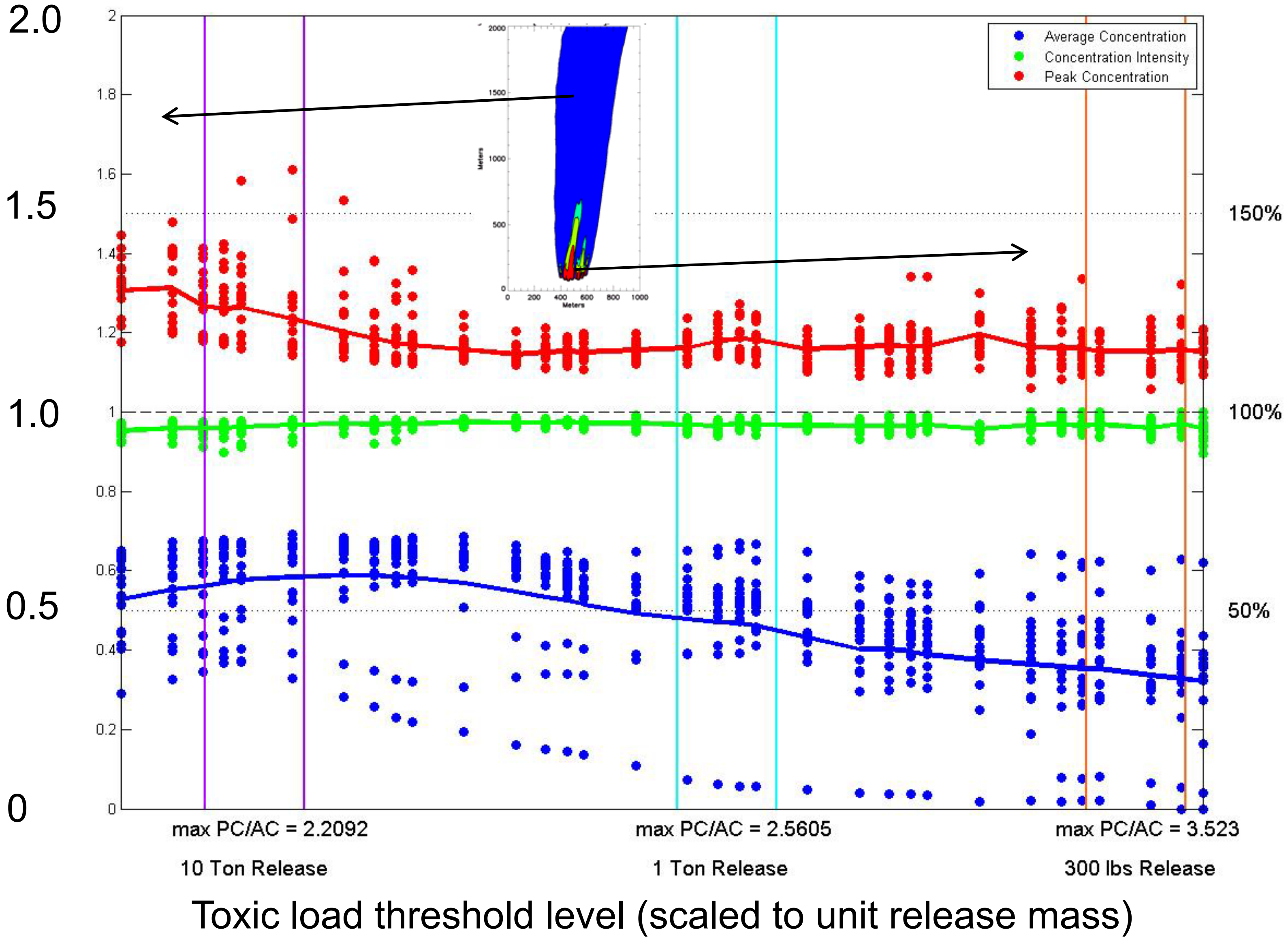


Max ratio between all models = 12.09

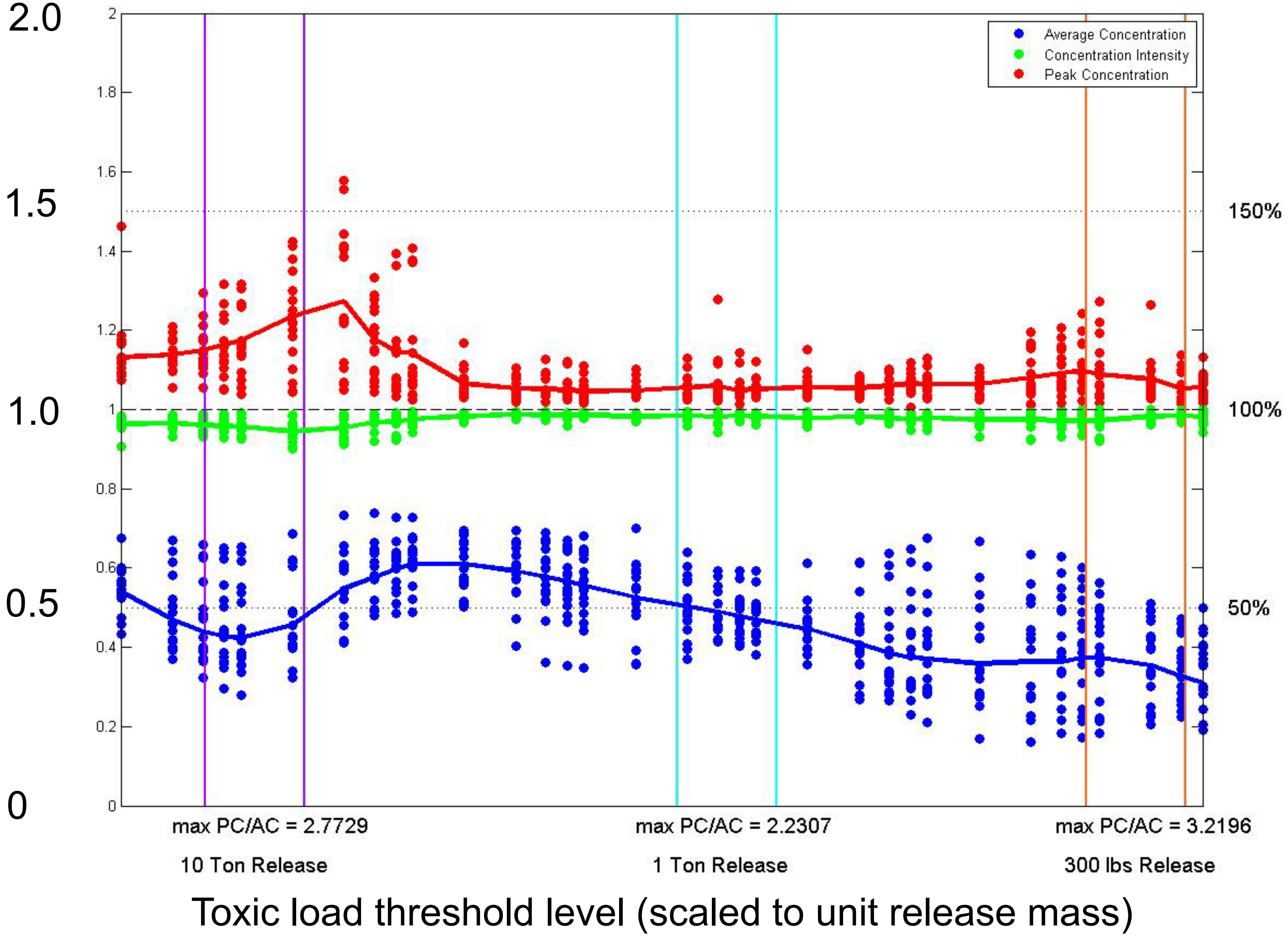
Threshold Area Relative to “tB” Threshold Area Neutral, All Sources



Ratio of “area above toxic load threshold” to “area above ten Berge toxic load threshold” (3 different toxic load models) – Multiple chlorine releases / Neutral stability



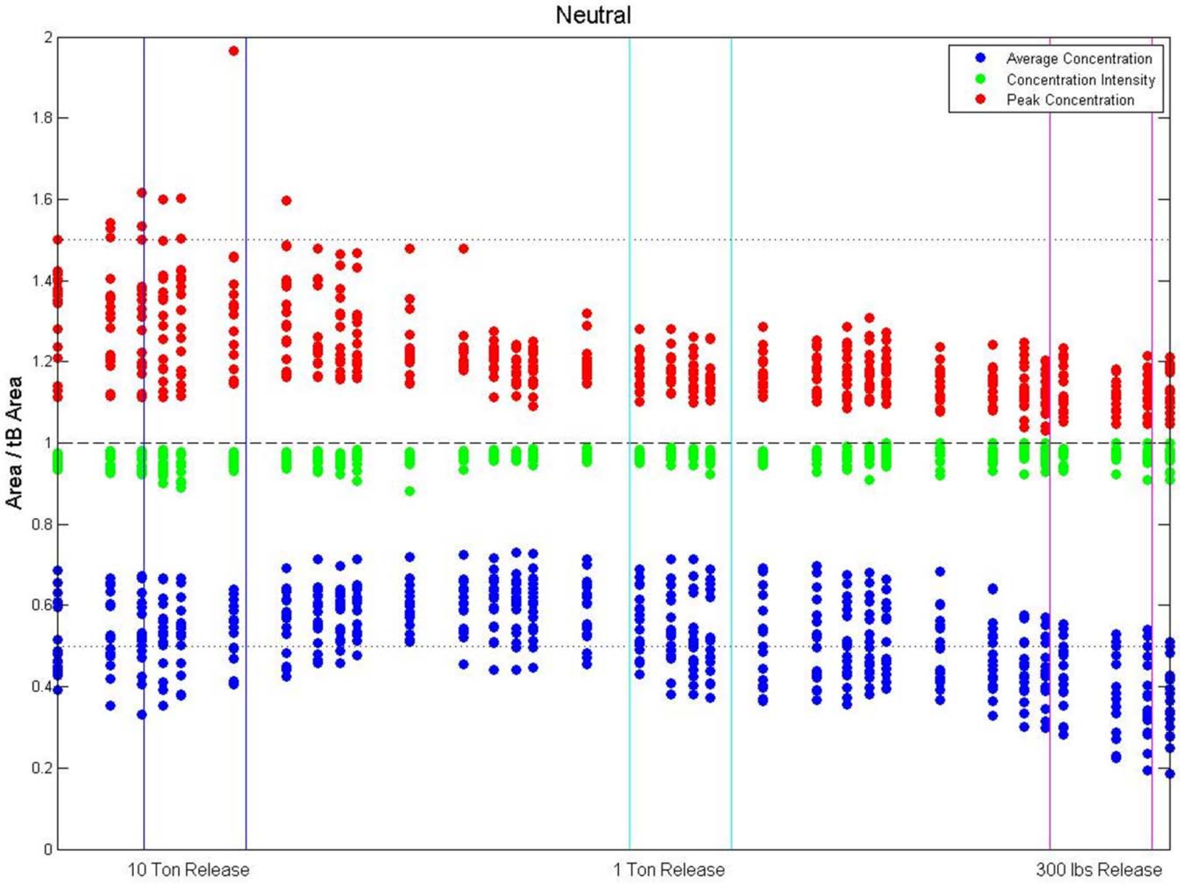
Ratio of “area above toxic load threshold” to “area above ten Berge toxic load threshold” (3 different toxic load models) – Multiple chlorine releases / Convective atmosphere



Toxic load model hazard area estimates for Chlorine

Neutral atmospheric conditions, <u>all 18 sources</u>

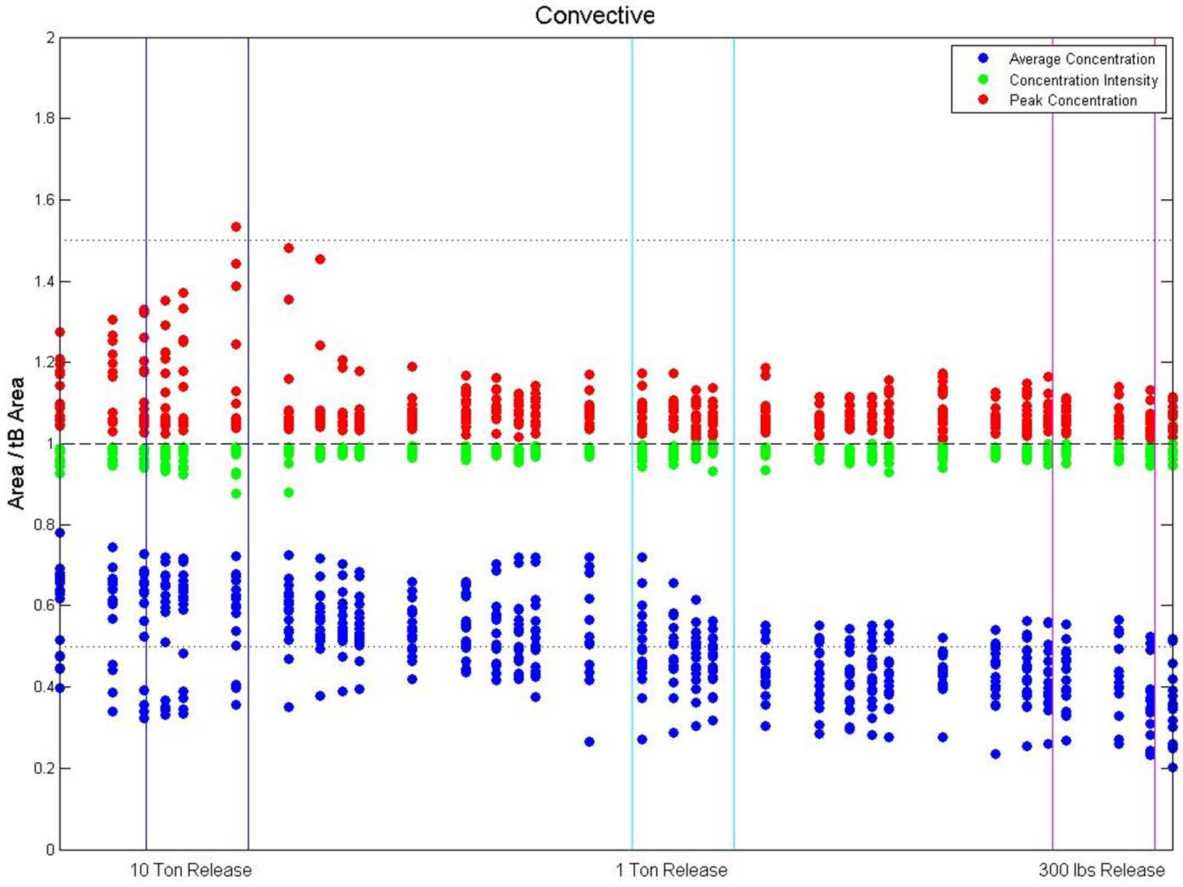
(Wind perpendicular to attack axis)



Toxic load model hazard area estimates for Chlorine

Convective atmospheric conditions, all 18 sources

(Wind perpendicular to attack axis)



Toxic load model hazard area estimates for Chlorine

All 18 sources

(Wind perpendicular to attack axis)

Release Mass, kg	Neutral Atmosphere		Convective Atmosphere	
	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