14th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
Kos Island, Greece
2-6 October, 2011

Use of Ensemble-Mean Plume versus Individual Plume Realizations for Toxic Load Modeling

IDA: Nathan Platt, Christopher Czech, Jeffry Urban, Dennis DeRiggi, Michael Ambrose

NCAR: Paul Bieringer, George Bieberbach, Andrzej Wyszogrodzki, Jeffrey Weil

Motivation – Transport and Dispersion (T&D) Modeling

Source Term
- ***Chem/Bio Weapon***
- ***Terrorist Attack***
  - ***Toxic Industrial Chemicals (TICs), radiological dispersion devices***
- ***Accident***
  - ***TICs***

Hazardous Plume Evolution
- ***Concentration/dosage in time and space***

- ***Casualty Estimation***

T&D

T&D modeling connects attacks or accidents to consequences/casualties

Applications
- ***Real Time***
  - ***Situational Awareness / Common Operating Picture***
- ***Non Real Time***
  - ***Planning***
  - ***Consequence Management***
  - ***Forensics***

Human Effects of Toxic Chemicals
Haber's Law and Dosage

- Different models have been proposed to relate a chemical concentration exposure profile to the toxic effect on humans.

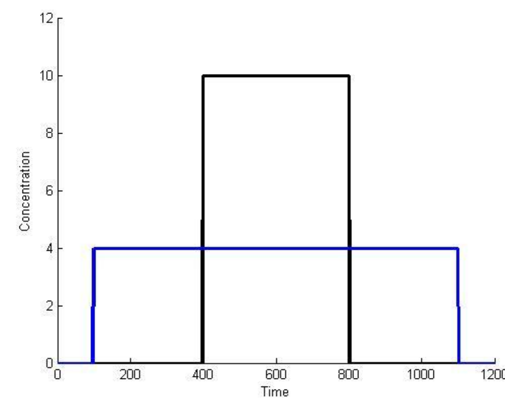
- Haber's Law and Dosage: $$D(\mathbf{x}) = C(\mathbf{x})T = \int_{t_{start}}^{t_{end}} C(\mathbf{x},t)dt$$

  - Haber's law is defined for constant concentration; temporal integration is an unverified (via experiments) generalization for time-dependent C(x,t)

- Haber's Law implies that resultant injury from exposure is independent of the manner in which the dosage was temporally accumulated

- Both long-exposure, low-concentration and short-exposure, high-concentration events result in same toxic effect. This is not true for all chemical agents, in particular chemical warfare agents.

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



Effects of Toxic Chemicals on Humans
Toxic Load Modeling and Toxic Load Exponent

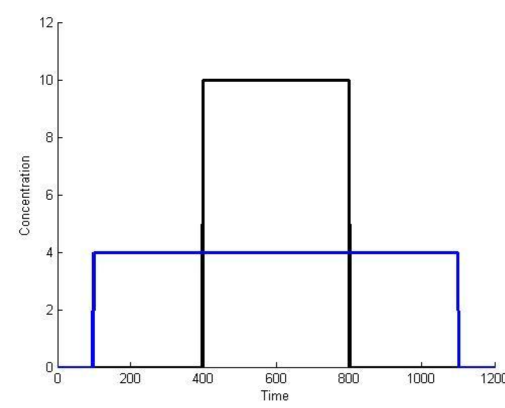
- A toxic load model of the following form has been suggested:

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

- Toxic load exponent *n* is determined by fitting experimental data
- Experimental data derived by measuring animal response based on fixed-duration, constant-concentration exposures
    - E.g., "rectangular" concentration pulses

- For *n*>1, a short-duration high-concentration "pulse" produces stronger toxic effects than a long-duration low-concentration "pulse"

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



Extension of Toxic Load Model to Time-Varying Concentration Exposures

- ten Berge (or Integrated): $TL(x) = \int c^n(\tau)\,d\tau$

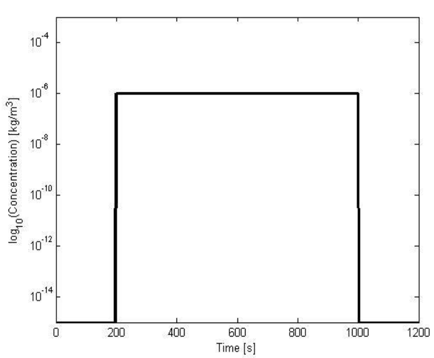
$$D = \int c(\tau)\,d\tau$$

- Average Concentration Method: $TL(x) = \left(\dfrac{\int_{t_{start}}^{t_{end}} c(\tau)\,d\tau}{t_{end} - t_{start}} \right)^n (t_{end} - t_{start}) = D^n T^{1-n}$

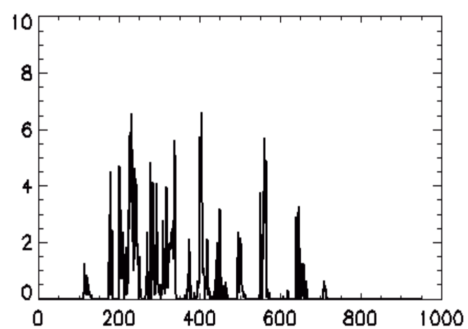
- Peak Concentration: $TL(x) = D^n T^{1-n}$ where $T = \dfrac{D}{C_{peak}}$; $TL(x) = \dfrac{D}{C_{peak}^{1-n}}$

- Conc. Intensity: $TL(x) = D^n T^{1-n}$ where $T = \dfrac{\left(\int c(\tau)\,d\tau\right)^2}{\int c(\tau)^2\,d\tau} = \dfrac{D^2}{\int c(\tau)^2\,d\tau}$; $TL(x) = \dfrac{D^{2-n}}{\left(\int c(\tau)^2\,d\tau\right)^{1-n}}$

Laboratory Testing Profile



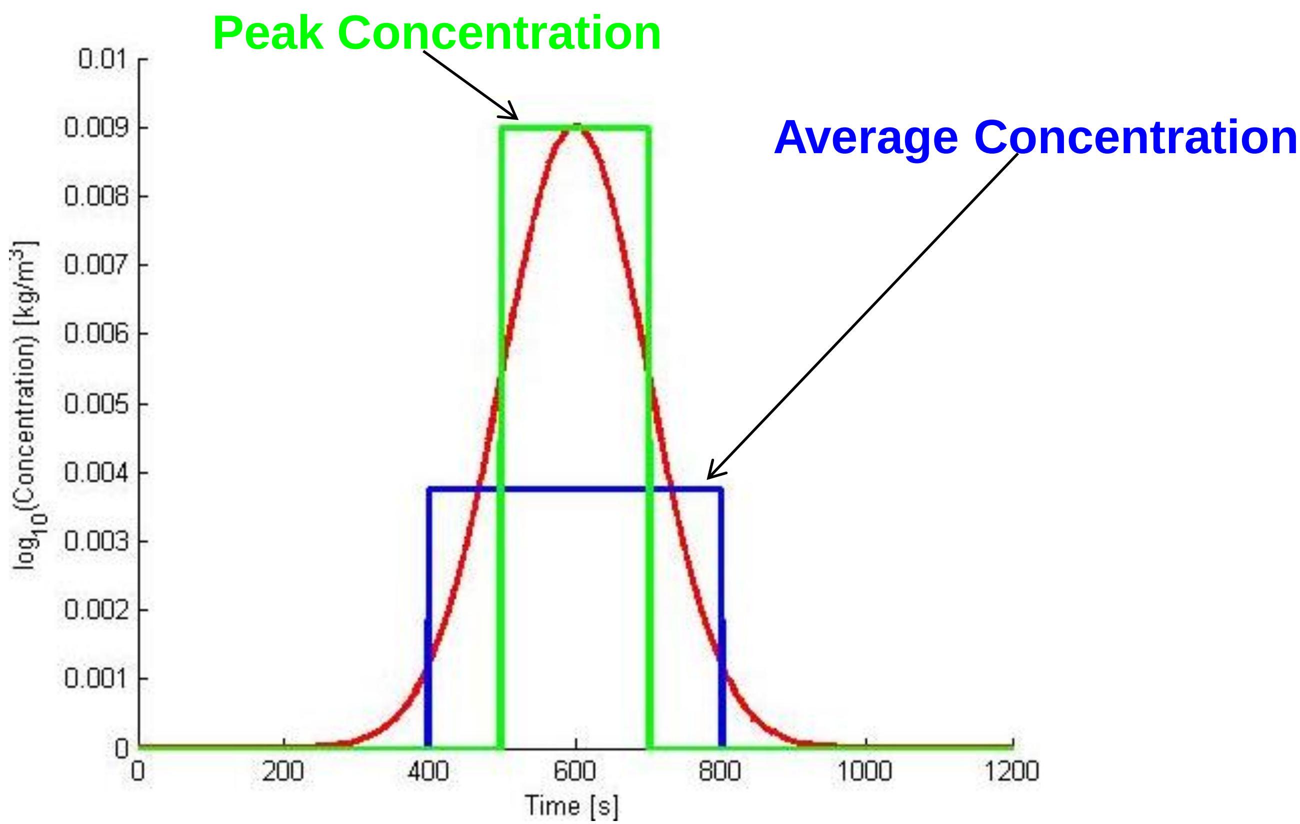
Possible Real-World Profile



For Peak Conc. and Conc. Intensity extensions, time *T* is sometimes called a generalized exposure duration

Concentration time history used to calculate ten Berge, Peak Conc. and Conc. Intensity toxic loads should be bin-averaged over some reasonable time interval equivalent to the duration of a single “breath” (e.g., 5-10 seconds)

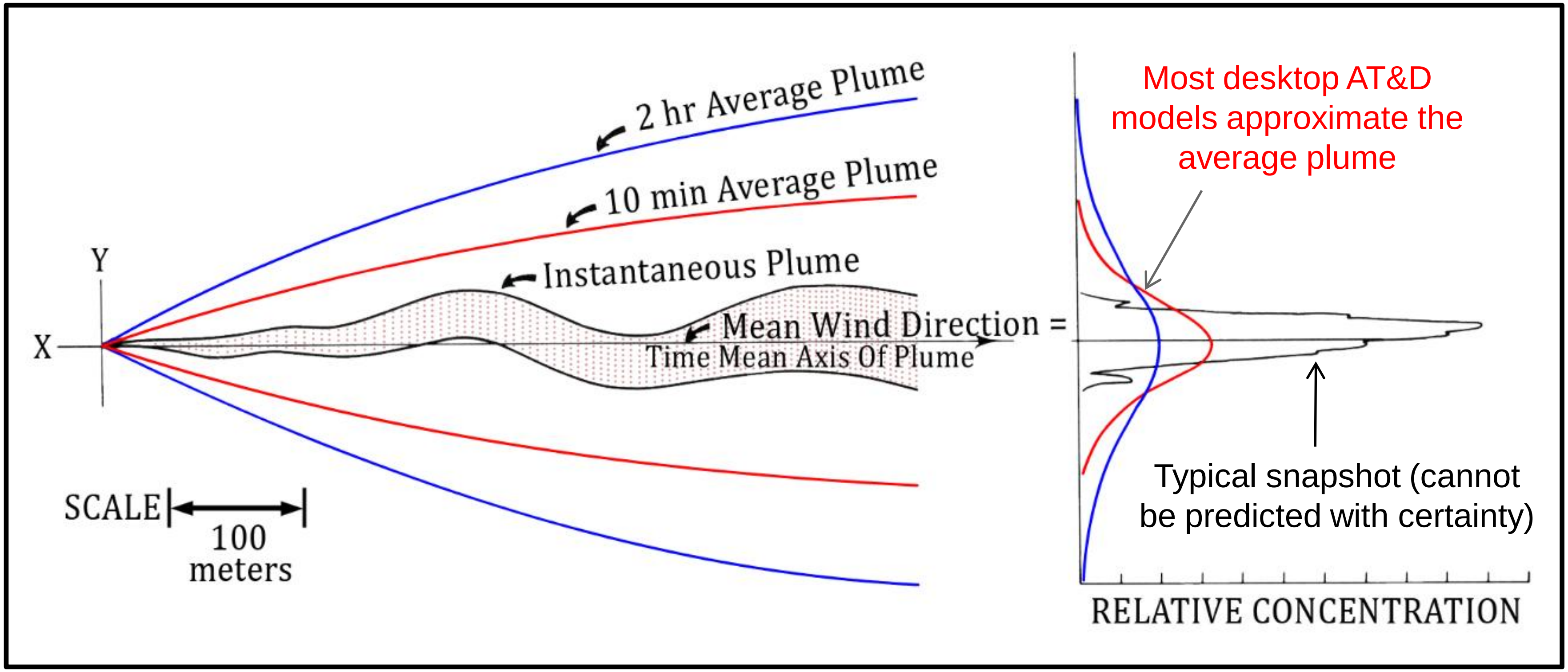
Notional Comparison of Average Concentration Model with Peak Concentration Extension



In some respects, the Average Concentration and Peak Concentration models capture two extremes in extending the toxic load model for a constant-concentration pulse to the case of time-varying concentrations

Mean Plume vs. Individual Realizations

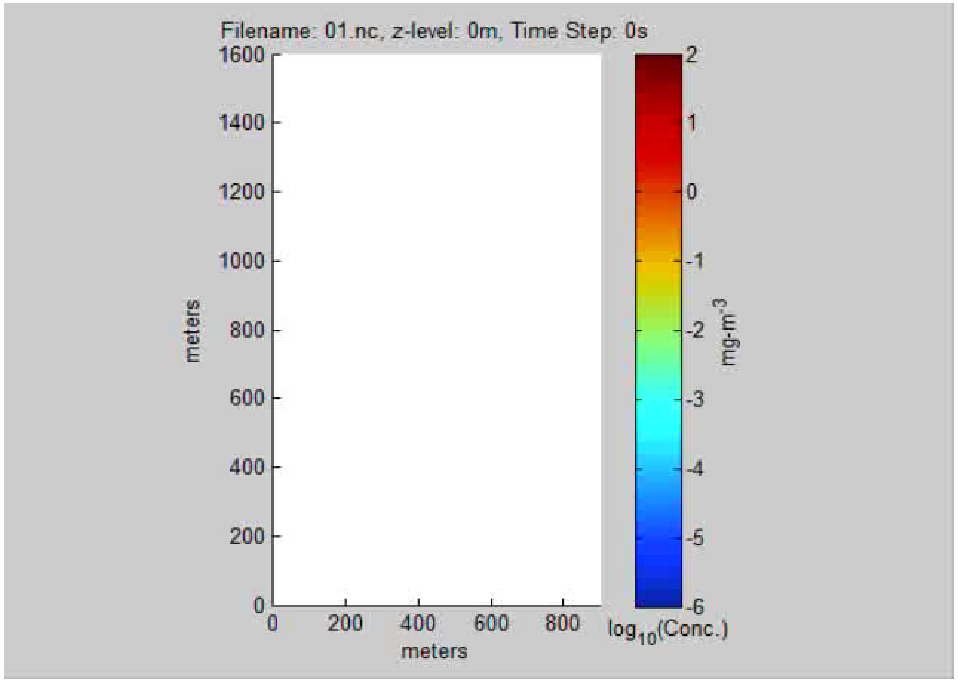
- **Most T&D models used in consequence assessment produce plumes that represent the ensemble average (mean) over turbulent realizations**



From presentation given by Dr. Paul E. Bieringer of the National Center for Atmospheric Research – June 22, 2010

Virtual THreat Response Emulation and Analysis Testbed (VTHREAT)

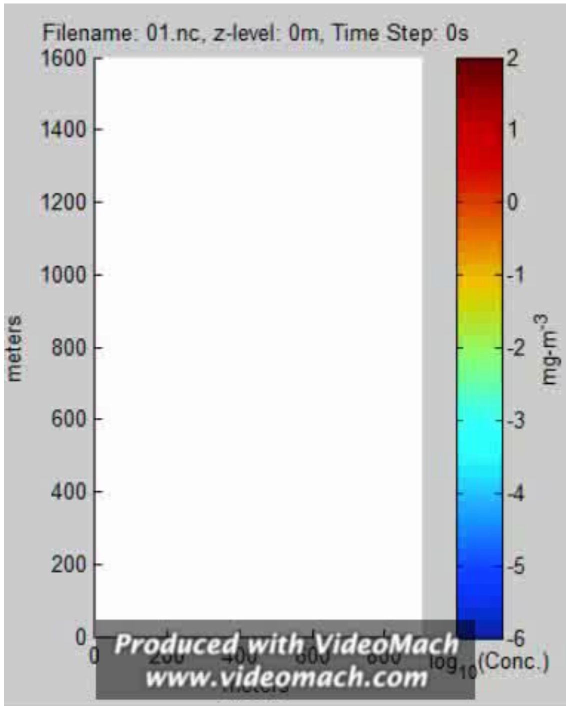
- VTHREAT is "a computational framework that utilizes a variety of research-grade atmospheric and T&D models to generate realistic 4-D representations of chemical and biological agent behavior in various turbulent atmospheric environments."
- A set of VTHREAT output files containing individual concentration realizations of FFT07 Trial 54 was generated to support validation of VTHREAT
    - 20 individual realizations
        - *0-, 5- and 10-meters vertical levels*
        - *1-sec temporal resolution*
        - *5 meters by 5 meters horizontal resolution*



Bieberbach et al.: Virtual CB agent data set generation to support evaluation of CB contamination avoidance systems

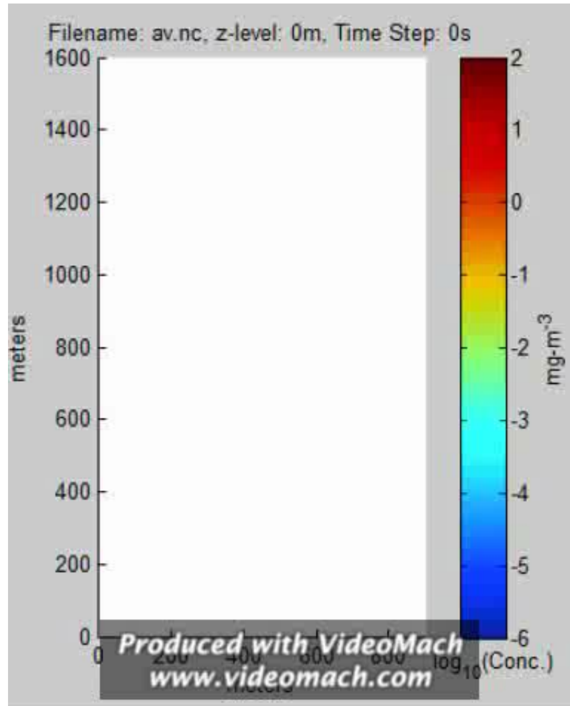
Individual Realization vs. "Mean Plume"

Construction of an "Ensemble Mean Plume"



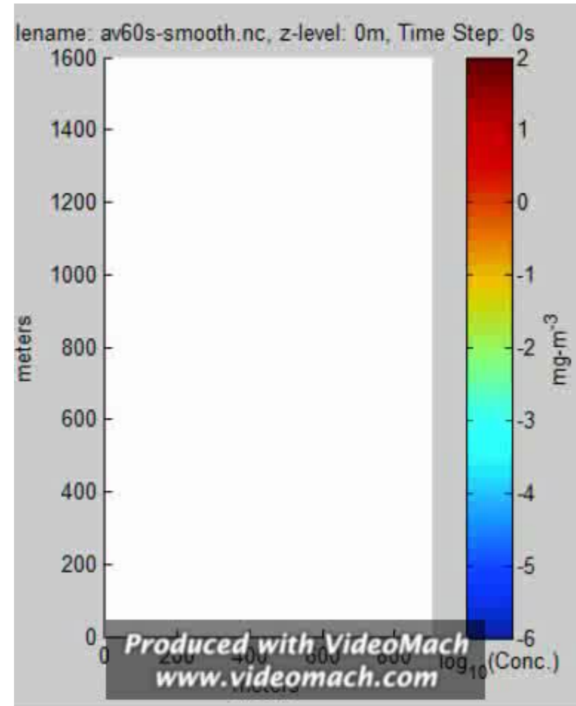
Individual Plume Realization

One of twenty different realizations of a simulated plume release.



Limited Ensemble Average

Constructed by averaging the concentrations of each individual plume realization, point by point



Temporally Averaged Ensemble Average

Constructed from the limited ensemble average with a 60-second running window average

The VTHREAT simulations used in this study represent relatively stable atmospheric conditions.

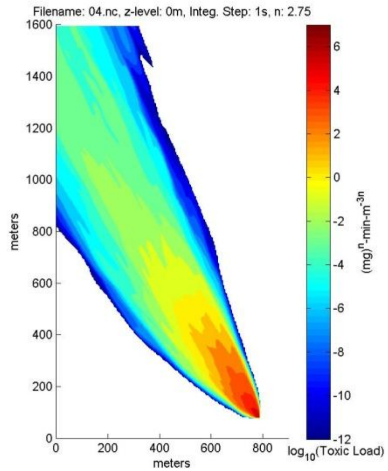
Understanding Time-Dependent Effects

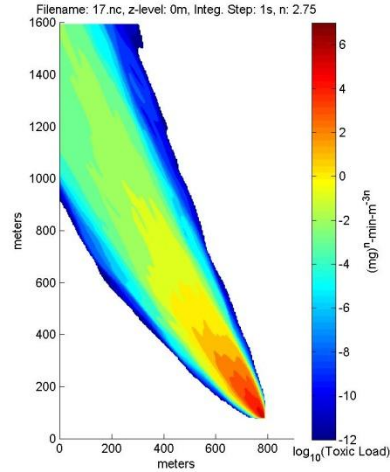
- Four different proposed toxic load models for time-varying concentration exposures were analyzed using the 20 individual realizations produced by VTHREAT on March 10, 2010.
  - Three different toxic load exponents
    - n = 1, 1.5, and 2.75

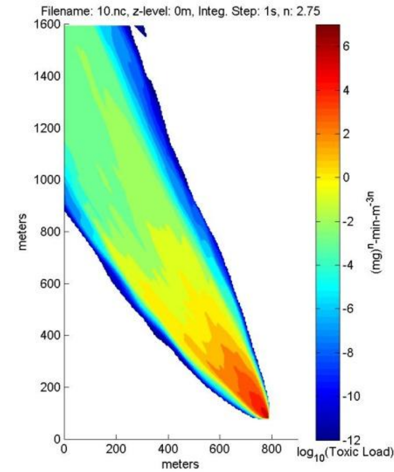
- **Question:**
  - **Within a given toxic load model, how do hazard areas predicted by individual realizations compare with those predicted by ensemble mean plumes?**

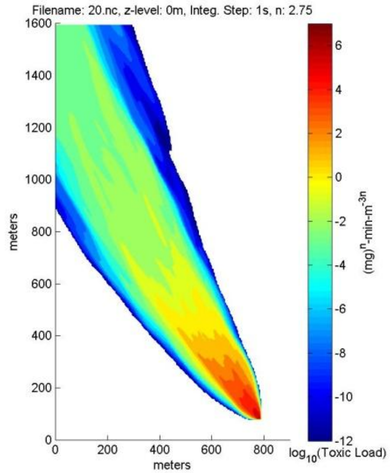
Comparing Individual Realizations with the Mean Plume

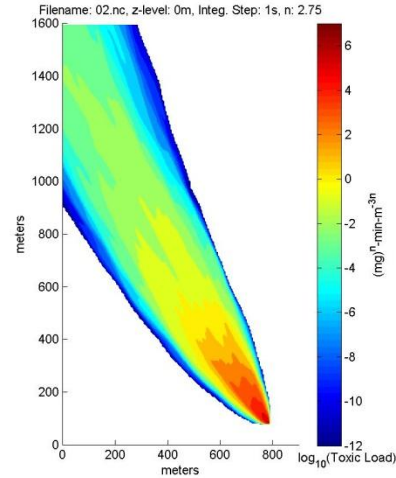
Integrated Toxic Load results

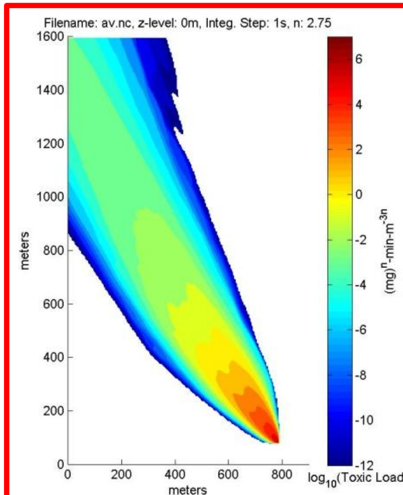












Establishing a Comparison Metric

<u>Procedure</u>

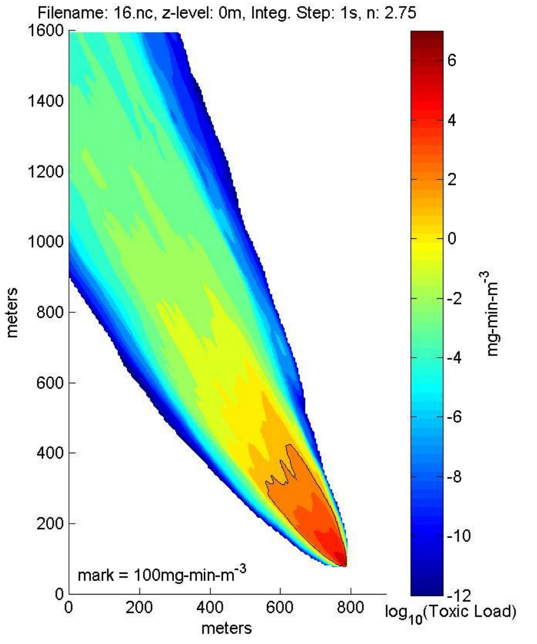
1. Choose a threshold toxic load value

2. Determine how much of the plot area [m^2] has a toxic load above that threshold value.

3. Repeat the process for different threshold values.

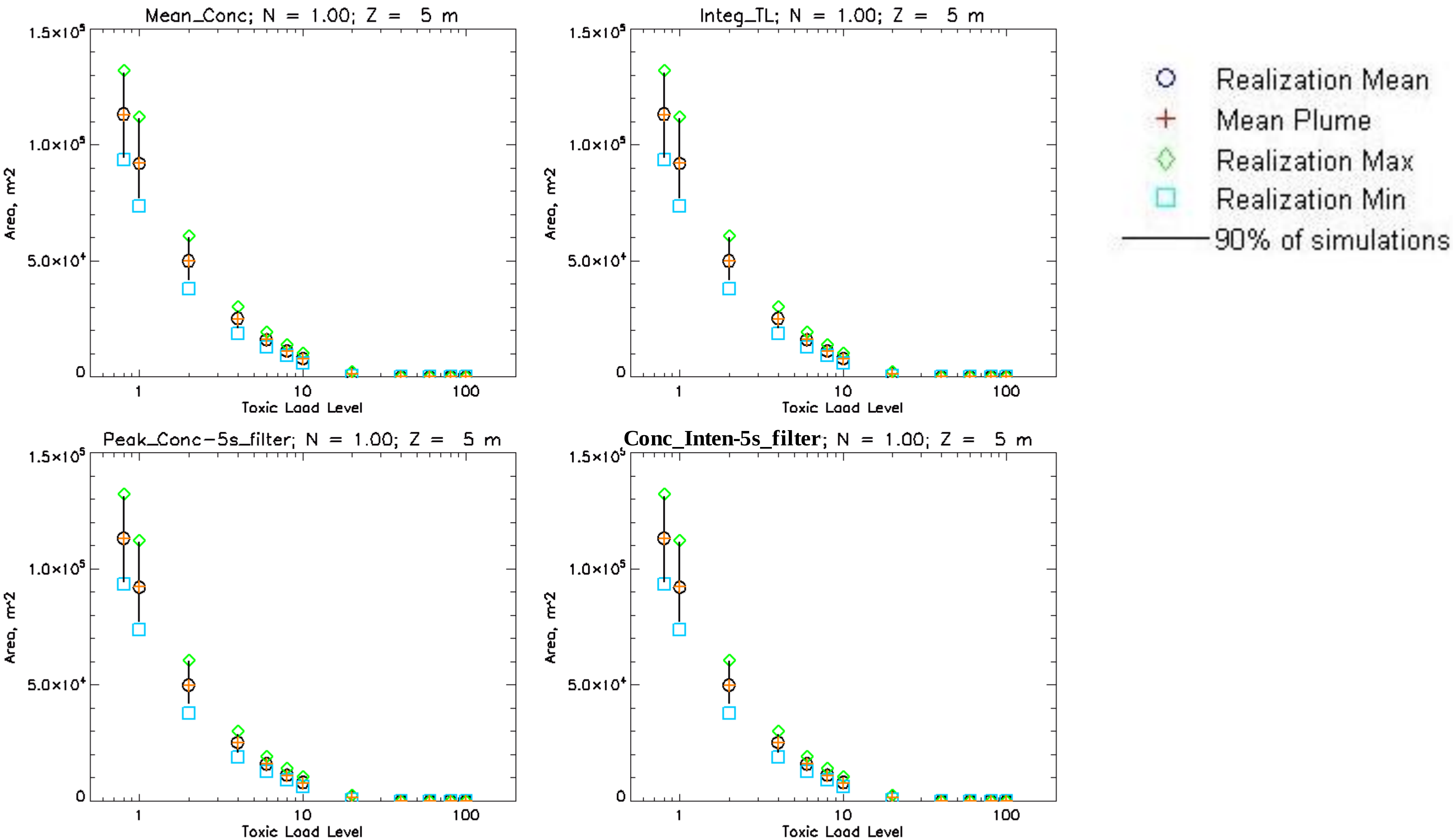
4. Repeat the process for each toxic load plume realization, and for the average toxic load plume.

5. Result is a list of "areas above threshold" as a function of threshold value.



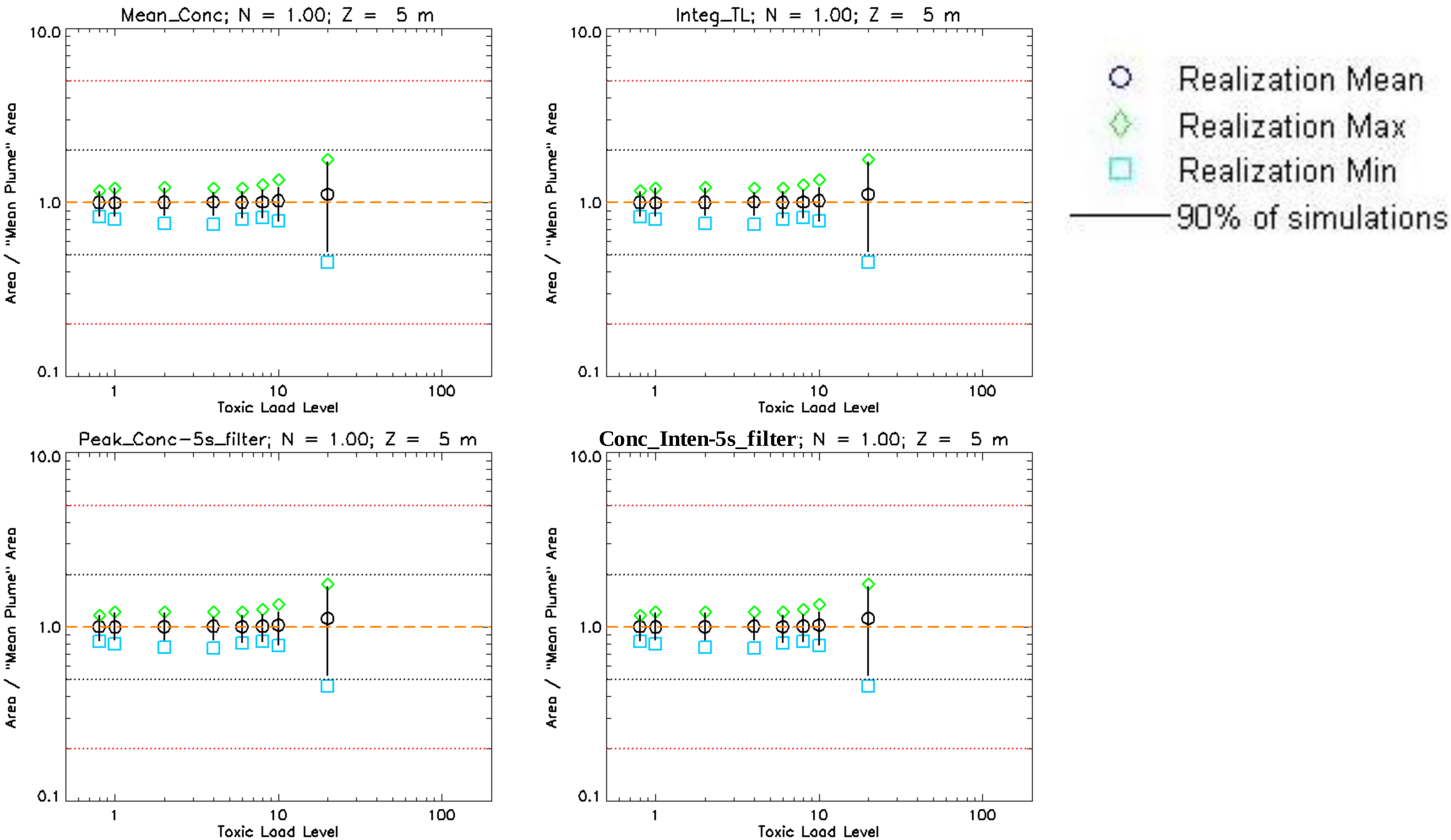
Toxic Load Threshold vs. Enclosed Area

N = 1, Z = 5 m



For *n* = 1 (Haber's law regime) , a wide spread in hazard areas is seen among the individual realizations, especially at low toxic load levels

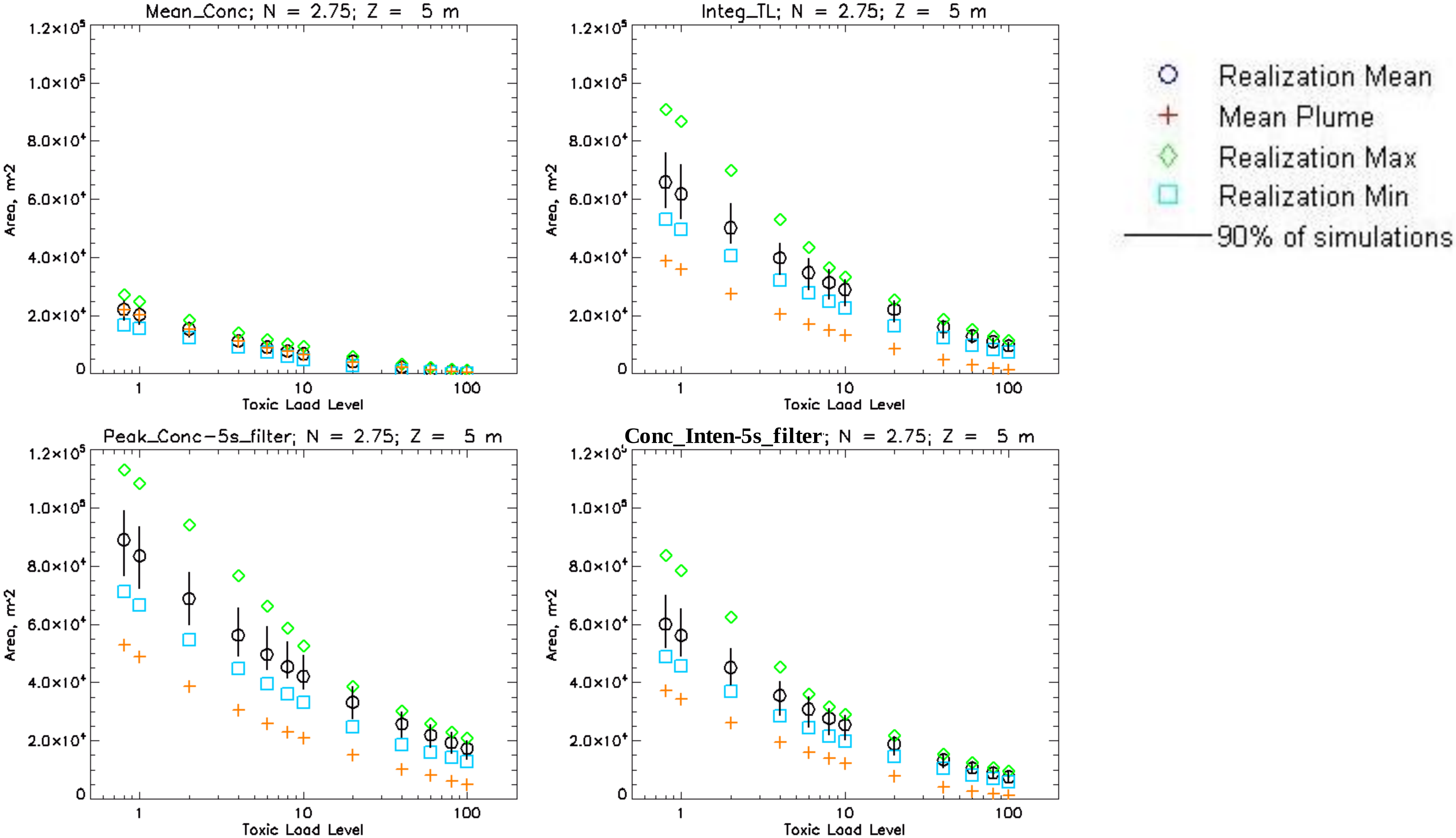
Toxic Load Threshold vs. Area / “Ensemble Mean Plume” Area
N = 1, Z = 5 m



For *n* = 1 (Haber’s law regime), the spread in the ratio of the toxic load area for individual plume realizations to the toxic load area for the “ensemble average plume” is approximately constant at all toxic load levels

Toxic Load Threshold vs. Enclosed Area

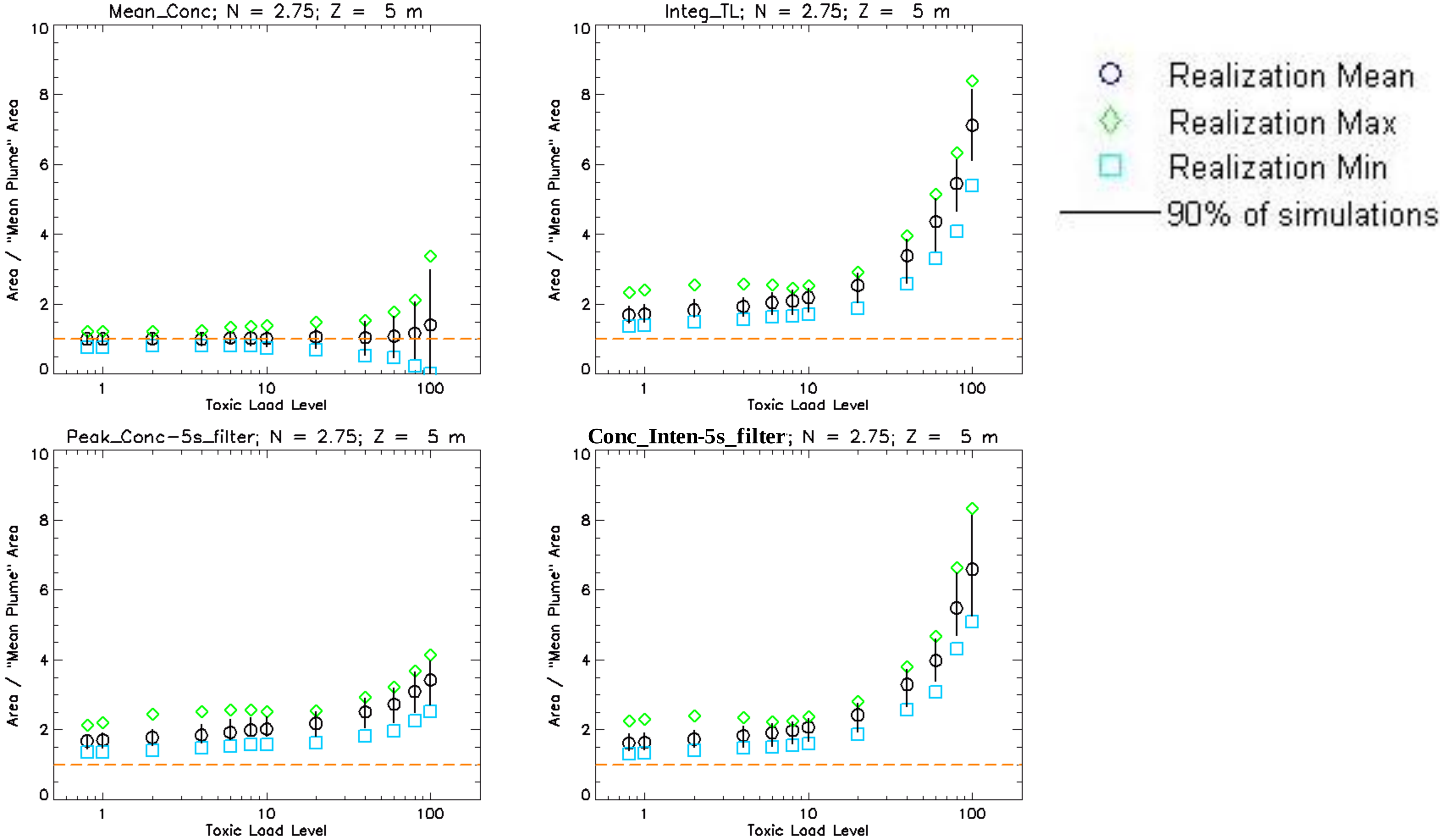
N = 2.75, Z = 5 m



For *n* = 2.75, with exception of "Average Concentration" method, all realizations have a significantly larger toxic load area than that of the "ensemble average plume"

Toxic Load Threshold vs. Area / "Ensemble Mean Plume" Area

N = 2.75, Z = 5 m



For *n* = 2.75, with the possible exception of the "Average Concentration" method,

- The spread in the ratio of the toxic load area for individual plume realizations to the "ensemble average plume" toxic load area increases significantly for higher toxic load levels
- The ratio of the average of toxic load areas for individual plume realizations to the "ensemble average plume" toxic load area increases significantly for higher toxic load levels

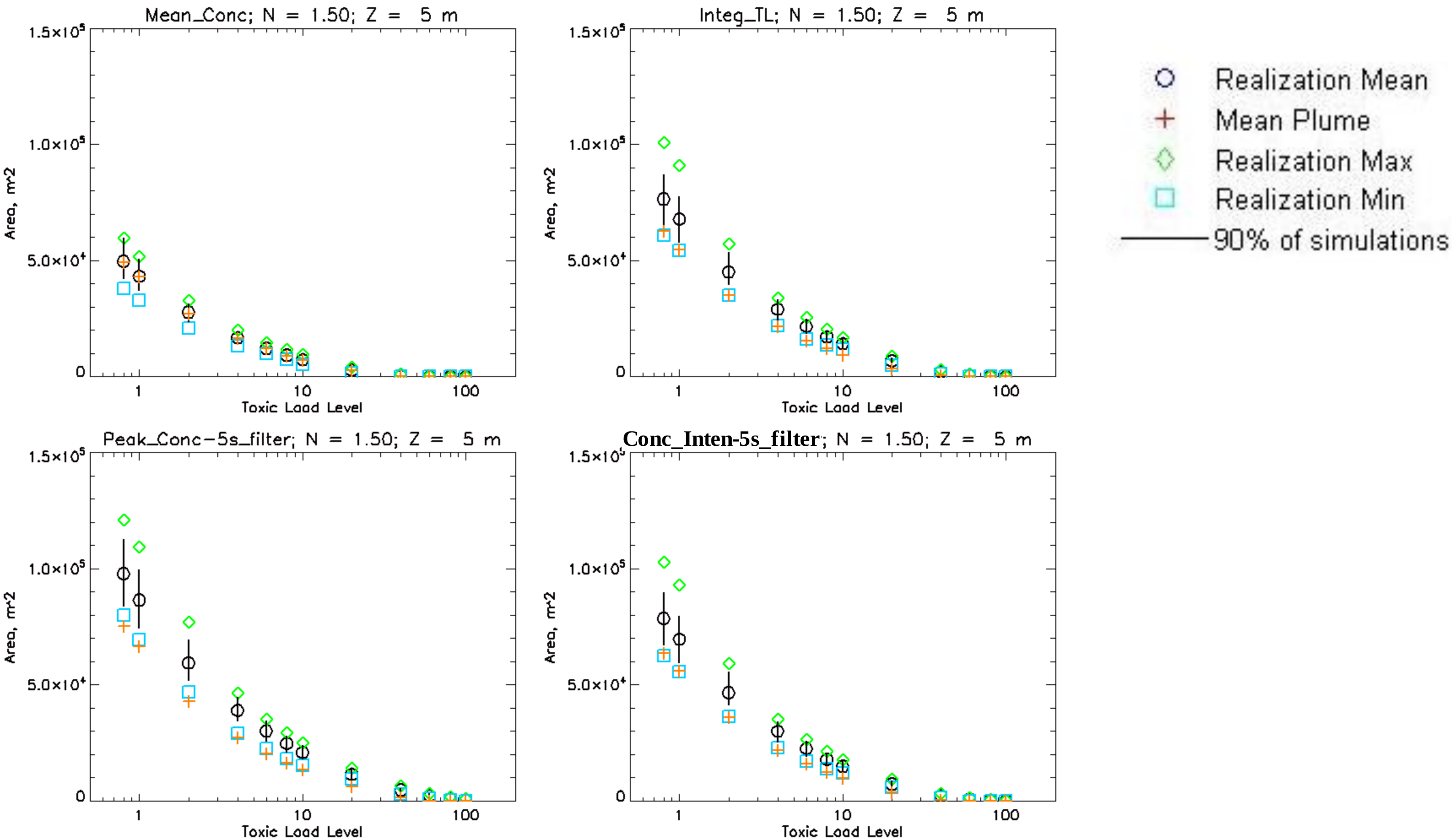
Conclusions

- Great care should exercised when toxic load modeling is applied to calculate consequences of the attack
- Most T&D models produce "ensemble average" plumes that smooth out concentration fluctuations in both space and time compared to actual realizations
- Most "real" plumes exhibit significant spatial and temporal fluctuations
- Toxic load models with a toxic load exponent greater than 1 magnify the effects of "localized" (both space and time) "hot zones", resulting in significantly larger hazard areas for individual plume realizations than for "ensemble average" plumes
  - At higher toxic load values, for which the most intense effects (e.g., deaths) are expected, the ensemble-average plume could *greatly under-predict* hazard areas.
  - We suspect that the use of common consequence assessment models, which produce ensemble mean plumes, in conjunction with toxic load modeling could greatly under-predict the consequences of a chemical release incident.
- Different extensions of the toxic load model extensions to the case of time-varying concentrations could produce different estimates of the hazard area and casualties
  - There is (almost) no experimental evidence to either validate or refute different extensions of the toxic load model for time-varying concentrations, but different extensions are presently being advocated or even used for consequence assessment modeling

Backup

Toxic Load Threshold vs. Enclosed Area

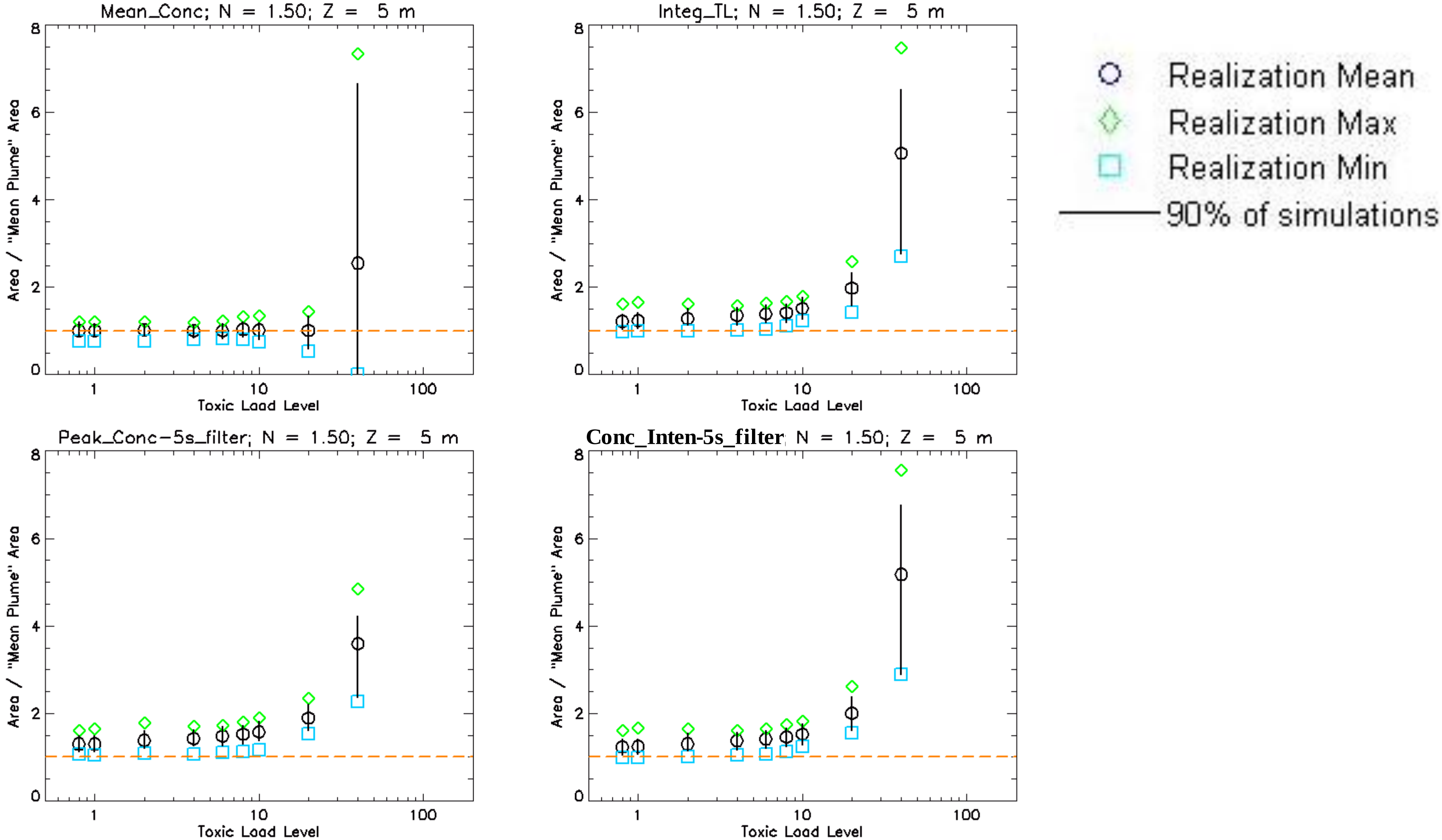
N = 1.5, Z = 5 m



For *n* = 1.5, with the exception of the "Average Concentration" method, almost all realizations have a larger toxic load area than the "ensemble average plume" toxic load area

Toxic Load Threshold vs. Area / "Mean Plume" Area

N = 1.5, Z = 5 m



For *n* = 1.5, with the possible exception of the "Average Concentration" method,

- **The spread in the ratio of the toxic load area for individual plume realizations to the "ensemble average plume" toxic load area increases for higher toxic load levels**
- **The ratio of the average of toxic load areas for individual plume realizations to the "ensemble average plume" toxic load area increases for higher toxic load levels**