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The Role of Atmospheric Dispersion Modelling in Modern Consequence Assessment Studies

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Introduction

- During the past 10+ years we have provided independent verification and validation of airborne hazard prediction models

- During this period, user needs for consequence assessment modeling capabilities have focused increasingly on *accurate* casualty predictions
  - Other applications, like prediction of hazardous areas, are still important

- Simultaneously, advances in consequence assessment modeling have raised hopes that accurate casualty prediction is possible
  - Higher spatial and temporal resolution atmospheric dispersion models, multiscale modeling, better population modeling, advanced toxicity models

- We recently have focused on examining whether the end-to-end combination of these modeling components is *consistent* and able to produce *accurate*, useful consequence assessments
  - These components must be assessed both individually and together in a user-oriented context

Obstacles to accurate casualty assessment

- Individual components of a hazard prediction model may be *inaccurate*
  - Uncertainties in source term modeling and atmospheric dispersion modeling have been discussed within the community, although not always communicated well (quantitatively) to the user
  - Uncertainties in health effects modeling and population modeling are less well understood within the community, and less often conveyed to the user
  - For example, we recently have focused on uncertainties associated with the use of toxic load models for casualty assessment
- The components of a hazard prediction model may be *inconsistent with each other* for a particular application of the model
  - That is, does it make sense to combine two or more modeling approaches for a given application?
  - A consistent obstacle to combining model components is incompatibilities in the order in which averaging (spatial, temporal, ensemble) occurs
  - For example, we recently have focused on the use of ensemble-mean atmospheric dispersion models in combination with toxic load models

IDA | Introduction to casualty prediction

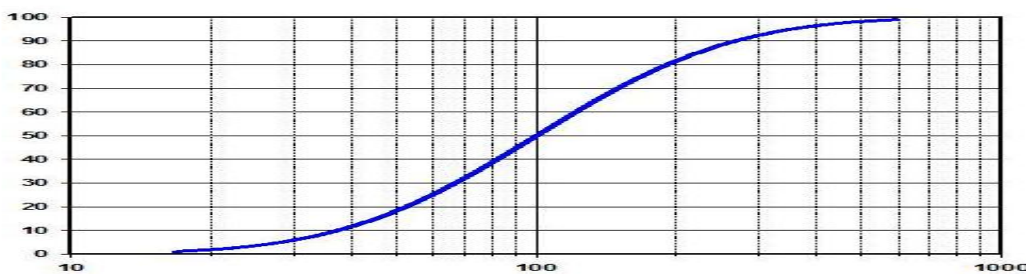
- The susceptibility of an individual to becoming a casualty is usually considered to be lognormally-distributed in the exposure (dosage)

- Probability of casualty at *r* is given by cumulative distribution function

$$P[D(r)] = \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{x_0} \exp\left[-(x-\mu)^2/(2\sigma^2)\right] dx \qquad x_0 = \log(D(r))$$

  - **Two toxicity parameters: μ (log(median effective dosage)) , σ (reciprocal of "probit slope")**

$P[D(r)]$



$\log[D(r)]$

- For a single deterministic dosage prediction, the total casualties are given by the population-weighted sum over all locations *r*

$$Cas\{P[D(r)]\} = \int P[D(r)]\ \rho(r)\ dr$$

  - ρ(*r*) = static population density

Haber’s Law and Toxic Load

- 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

- Real-world exposures (and most dispersion model outputs) do not involve steady concentrations

- An *unproven* generalization for time-varying exposures is

$$D(r) = \int_0^T c(r,t)\,dt$$

- 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

- One (*unproven*) generalization (of *many*) for time-varying exposures is

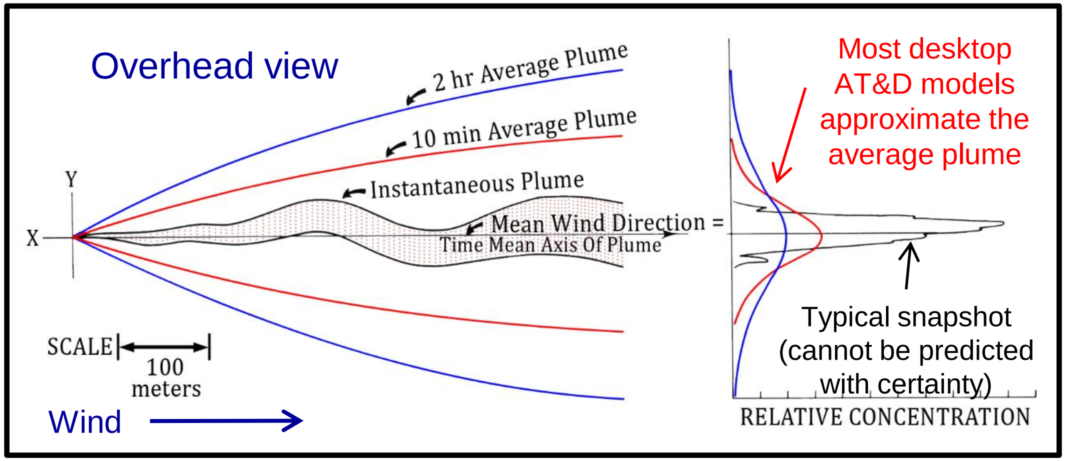
$$TL(r) = \int_0^T [c(r,t)]^n\,dt \qquad \text{(ten Berge model)}$$

The problem with ensemble averaging

- Most hazard prediction models output only the ensemble average over concentration realizations rather than individual realizations

- Ensemble-averaging smoothes out the plume in time and space

- Even if the distribution of concentration realizations is known, the distribution of casualties may not be



Adapted from presentation given by P. Bieringer , U.S. NCAR (22 June 2010)

Intuitive way of calculating casualties from ensemble mean *c*(*r*,*t*):

$$\overline{c(r,t)} \to D[\overline{c(r,t)}] \to P\{D[\overline{c(r,t)}]\} \to Cas[P\{D[\overline{c(r,t)}]\}] \neq \overline{Cas[P\{D[c(r,t)]\}]}$$

$$\overline{c(r,t)} \to TL[\overline{c(r,t)}] \to P\{TL[\overline{c(r,t)}]\} \to Cas[P\{TL[\overline{c(r,t)}]\}] \neq \overline{Cas[P\{TL[c(r,t)]\}]}$$

What is possible using only ensemble mean *c*(*r*,*t*)

What users need

Ensemble averaging – the dosage (Haber's law) problem

- Relating the ensemble distribution of concentration realizations to the ensemble distribution of dosage realizations is *not* straightforward
  - $c(r,t)$ distribution = clipped-normal, gamma, etc. $\rightarrow$ $D(r)$ distribution = ???

- We have demonstrated a relationship under certain conditions:
  - Variance of concentration fluctuations is small compared to the mean
    - **Implies, via central limit theorem, that *D*(*r*) is normally-distributed**
  - The concentration fluctuation autocorrelation decays exponentially with *t*
    - **This permits the calculation of the variance of the normally-distributed *D*(*r*)**
  - Concentration fluctuations are clip-normally distributed

- Given these conditions, the distribution of dosages can be calculated from the ensemble mean concentration *and its variance*
  - Most atmospheric dispersion models do not output concentration variance
    - **An exception is the SCIPUFF model (used in HPAC)**

- If the distribution of dosages is known, the ensemble mean number of casualties and its variance can be calculated

Ensemble averaging – the toxic load problem

- Relating the distribution of concentrations to the distribution of toxic loads is harder than it is for dosages, due to the concentration exponent

- We have not yet found a way to calculate toxic load derived casualties directly from low-order moments of the concentration ensemble
  - Even a full moment expansion loses the spatiotemporal correlations
  - Even calculating toxic load hazard areas (ensemble mean toxic load) is challenging – depends on the form of the toxic load model (ten Berge is OK)

- Our prior work suggests that using the ensemble average plume directly with toxic load models ($n > 1$) can underestimate casualties significantly
  - Ensemble averaging smoothes out harmful concentration spikes

- The concentration exponent in toxic load models also causes problems in terms of time averaging (similar to problems w/ ensemble averaging)
  - Introduces an undetermined “concentration pre-averaging timescale”
    - **Lower bound of averaging time is probably the human respiration timescale, but the “correct” averaging time is not known (will depend on the hazardous material)**
    - **Some users choose averaging time from dispersion model outputs, not toxicity**

Toxic load modeling challenges – choice of toxic load model

- As discussed in the talk by Platt et al., it is not obvious how to generalize the toxic load model to the case of time-varying exposures

- Several generalizations have been proposed in the literature
  - None are well-supported by experimental data
  - Some seem to have been suggested principally on the basis of ease of use with particular atmospheric dispersion model outputs

- Our prior analysis of observations and simulations of a short-range dispersion field experiment indicate that the differences between toxic loads predicted by these models can be substantial

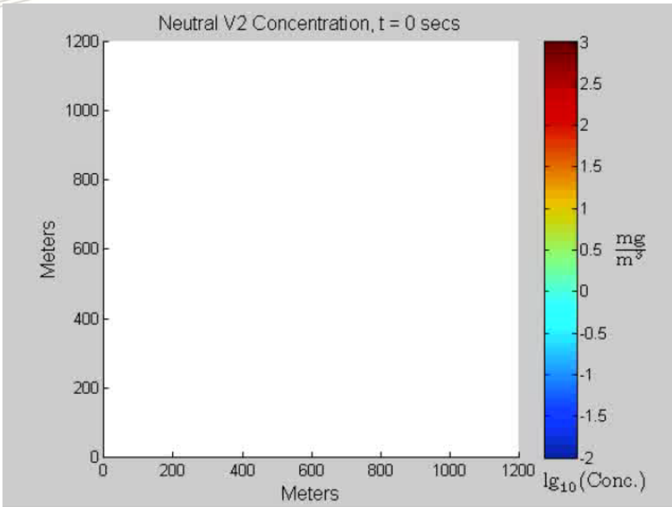
- We have recently analyzed simulations of realizations of a realistic chemical attack using real toxicity parameters for different chemicals
  - This provides a context for whether the differences matter at concentrations that correspond to lethal effects

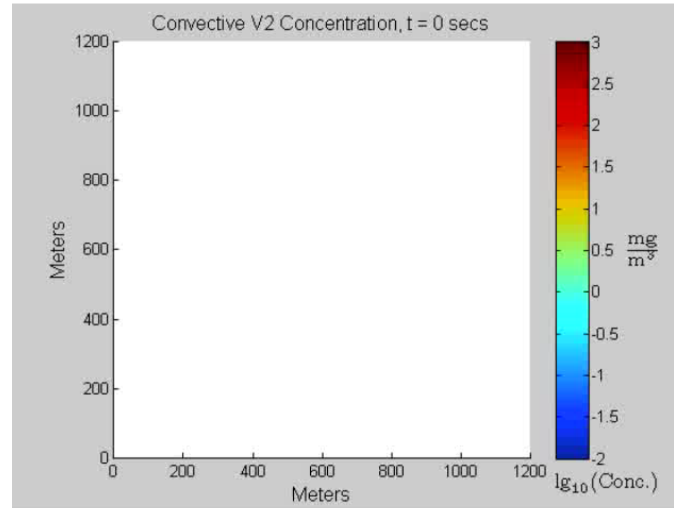
Choice of toxic load model – VTHREAT simulations

- We used results from NCAR’s VTHREAT simulation environment to generate four realizations of a chemical attack
  - 18 instantaneous sources intended to simulate a chemical artillery attack
    - **Sources spread over a 100 m × 200 m impact area**
  - Two atmospheric stability conditions (neutral, convective)
  - Two release geometries (attack axis along-wind or cross-wind)
  - Have not yet simulated an ensemble of realizations

- Investigated toxic effects using toxicity parameters of a chemical warfare agent (not shown in this presentation) and chlorine
  - For chlorine, we considered each source as a separate release and scaled the release size to 136 kg (2 150-lb. cylinders), 1 ton, or 10 tons
    - **Examined toxic load contours over the 1% lethal to 99% lethal range**
  - VTHREAT simulations were of a neutrally-buoyant gas – we are ignoring the (substantial) chlorine dense gas dispersion effects
  - Note: many chemical warfare agents have very high probit slopes, so toxic effects vary suddenly across plume (all dead or none)

VTHREAT-simulated chemical attack





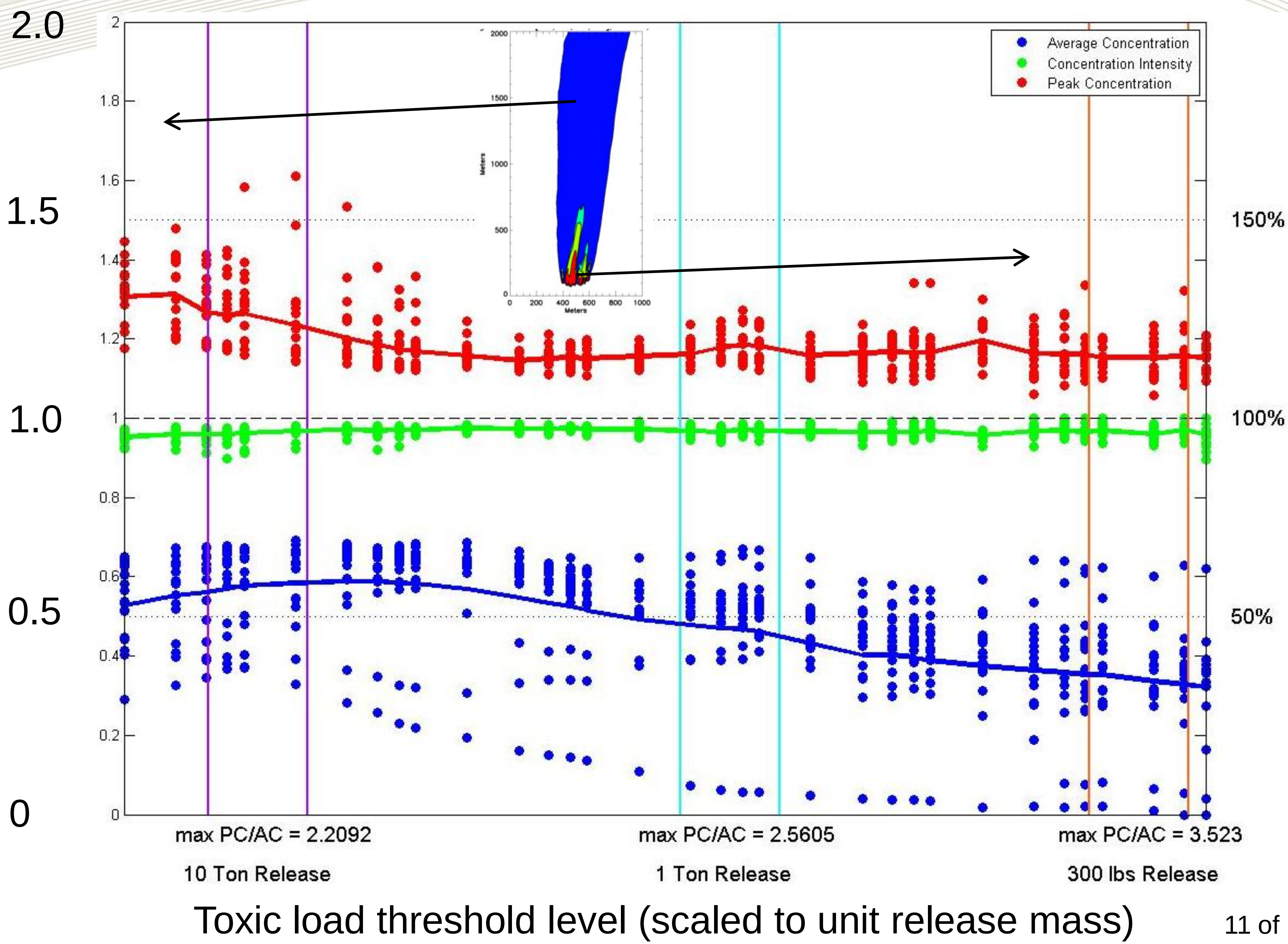
Neutral

Convective

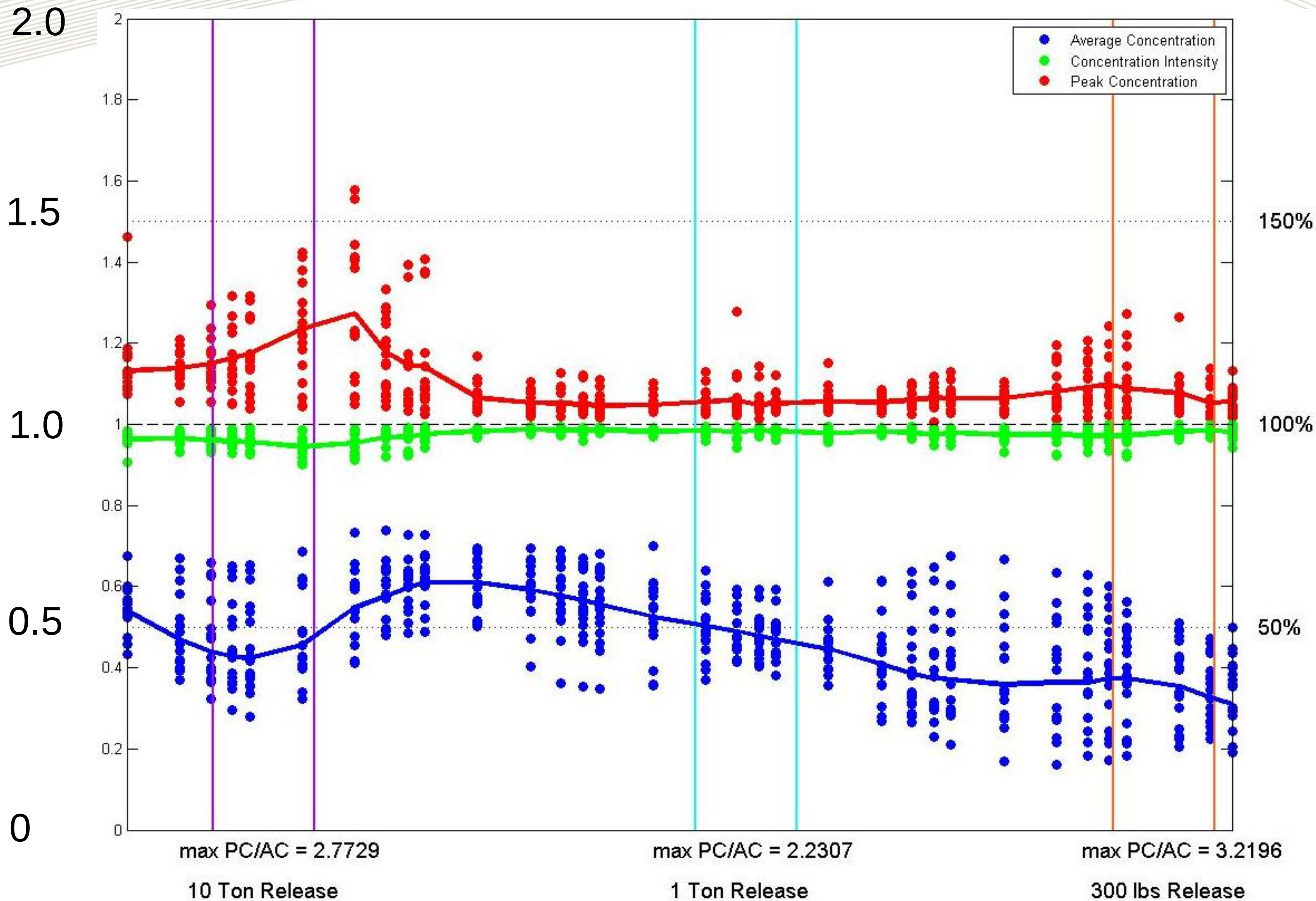
Long axis of source distribution perpendicular to wind

Contours indicate different concentration levels

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 threshold level (scaled to unit release mass)

VTHREAT-simulated chlorine attack – Observations

- The size of *hazardous areas* over which lethal effects vary between the 1% and 99% level *vary by a factor of 2 to 3* between the highest-predicting toxic load model (peak concentration model) and the lowest-predicting model (average concentration model)
  - Have not yet calculated casualty ratios for chlorine

- The magnitude of the variation depends not only on which source is considered (individual variability) but also the release size and the toxicity of the hazardous material
  - No obvious trends deduced yet

- Note: we have not yet examined a true ensemble of instantaneous sources – the variation between toxic load models could be different if we examine true individual realizations
  - The dispersion of our 18 instantaneous sources is somewhat correlated due to the spatial proximity of the sources

Modern consequence assessment – Other issues [1]

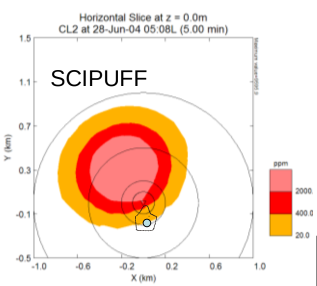
- Toxicological experiments sometimes yield a very large uncertainty in the derived toxicological parameters
  - This uncertainty is not typically propagated in consequence assessment studies or communicated to users

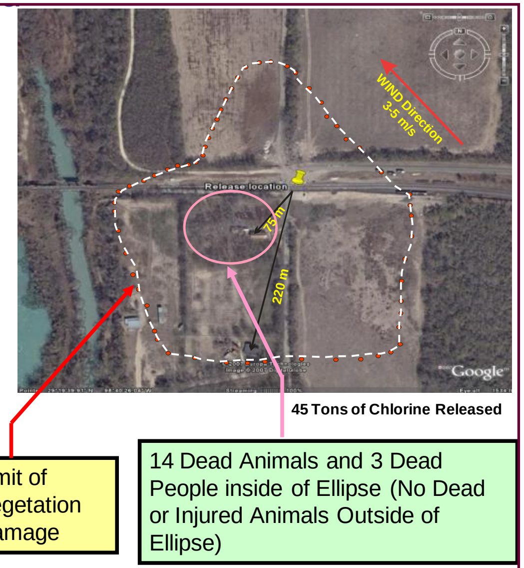
- Uncertainties in the population distribution are often poorly characterized
  - Also, using high spatial resolution dispersion model outputs with low resolution population data could result in inaccurate casualty estimates

IDA | Modern consequence assessment – Other issues [2]

- There is a feeling within the consequence assessment community that the consequences of real-world hazardous releases are overpredicted
  - Based almost entirely on overt chlorine releases (accidental and intentional)
  - Effects of evacuation and sheltering could be important; poorly understood
    - **Metric is often "distance from source where people died vs. distance where lethal concentration predicted", but rarely know population behavior – or actual concentrations**
  - Need to understand effects of microscale variation in terrain (dense gas gravity effects), land cover (vegetative filtration), population heterogeneity
  - Would be useful to consider other types of chemicals (e.g., ammonia accidents) or less overt releases (e.g., Bhopal) with modern models

Distance from Spill, (m)	Concentration Predictions from 6 Dispersion Models: Mean Concentration of Chlorine, (ppmv)	Range Concentration of Chlorine, (ppmv)
100	71,300	8,100 to 138,000
200	33,950	4,600 to 58,000
500	9,400	2,600 to 28,000
1,000	3,020	1,300 to 6,900
2,000	633	390 to 1,900
5,000	98	10 to 110





2004 chlorine railcar accident in Macdona, Texas

Observed casualties and vegetation damage vs. SCIPUFF prediction

Adapted from presentation given by Shannon Fox, U.S. DHS Chemical Security Analysis Center, 2009 GMU Conference on AT&D Modeling

Summary and recommendations [1 of 2]

- Using low-order ensemble moments (mean, etc.) of the concentration in toxicity models can produce inaccurate casualty estimates
  - Dosage is potentially problematic, toxic load more so

- Toxic load modeling, although touted as more accurate, has drawbacks
  - Notably, the aforementioned problem with ensemble-mean concentrations
  - No validated method of extending the model to the case of time-varying concentrations (competing models can disagree significantly)
  - Extra toxicity parameters (exponent, time averaging) – effect on uncertainty?
  - Possible that the more advanced toxicity model could give worse results??

- The uncertainties in toxicity modeling and population modeling (distribution, movement, sheltering) are not always well understood
  - Analytical uncertainties also are not always communicated to model users and the consumers of modeling products

Summary and recommendations [2 of 2]

- Health effects modeling and population modeling should be recognized as potentially critical contributors to consequence assessment studies
  - Less well understood than physics-based modeling, but not less important
  - If inaccurate or misleading, may reduce confidence in entire model
    - **In some cases, (ensemble) dispersion modeling may not be the dominant source of error**
- Consequence assessment models may need better treatment of concentration fluctuations, toxic effects, & population statics and dynamics
  - Even if experiments are not possible, theoretical and parametric studies can be used to bound the problem for decision-makers
  - Some recent U.S. experiments (micro-terrain/dense gas, time-varying toxicity)
- Modeling should be viewed as an end-to-end process
  - True even if consequence estimation performed outside of dispersion model
  - Propagation of uncertainty should be tracked from start to finish
    - **The order in which spatial, temporal, and ensemble averaging occurs is important**
  - *Harmonisation* is necessary to ensure that the end-to-end effort makes sense and that nothing is overlooked due to diffusion of responsibility
    - **Model developers (dispersion, consequence assessment) must work with model users, model evaluators, and consumers of modeling products**

Backup

Some proposed extensions of the toxic load model to the case of time-varying concentrations

- ten Berge (or Integrated): $TL_{ten\ Berge}(r) = \int c^n(r,t)dt$

- Average Concentration: $TL_{AverConc}(r) = \left(\frac{\int_{t_{start}}^{t_{end}} c(r,t)dt}{t_{end} - t_{start}} \right)^n (t_{end} - t_{start}) = D^n T^{1-n}$

- Peak Concentration: $TL_{PeakConc}(r) = D^n T^{1-n}$ where $T = \frac{D}{c_{peak}}$; $TL_{PeakConc}(r) = \frac{D}{c_{peak}^{1-n}}$

- Concentration Intensity: $TL_{ConcInten}(r) = D^n T^{1-n}$, where $T = \frac{\left(\int c(r,t)dt\right)^2}{\int c^2(r,t)dt} = \frac{D^2}{\int c^2(r,t)dt}$

$$TL_{ConcInten}(r) = \frac{D^{2-n}}{\left(\int c^2(r,t)dt\right)^{1-n}}$$

Here r is the location of the exposure, $c(r,t)$ the concentration time series at r, $D \equiv D(r) = \int c(r,t)dt$ is the accumulated dosage at r, and n is the toxic load exponent

Concentration averaging time – potential effects on inputs to toxic load models

FUSION Field Trial 2007 (FFT 07) Release 54, Sampler 78
10-minute morning release of propylene gas