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15th International Conference on Harmonisation within
Atmospheric Dispersion Modelling for Regulatory Purposes
6-9 May 2013
Madrid, Spain

The Use of Probabilistic Plume Predictions for the Consequence Assessment of Atmospheric Releases of Hazardous Materials

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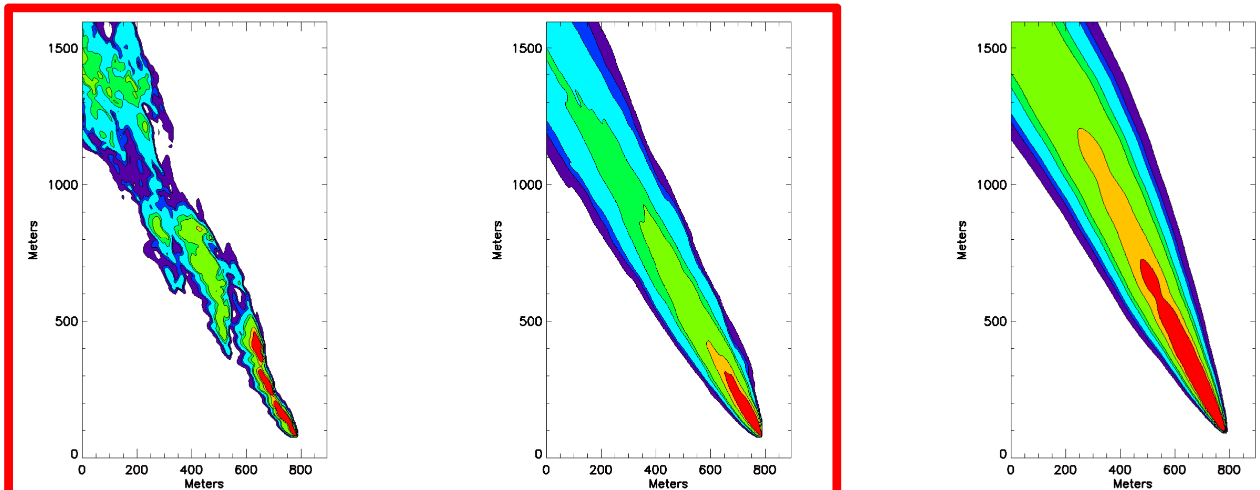
6 May 2013

Hazard Assessment Predictions Capability (HPAC) / Joint Effects Model (JEM)

- 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
- Second Order Closure Integrated Puff model (SCIPUFF) is a Langrangian Gaussian puff dispersion model that in addition to calculating mean field concentration also calculates concentration variance. HPAC outputs include pair $(\overline{c(\mathbf{x},t)}, \overline{c'^2(\mathbf{x},t)})$ or $(\overline{d(\mathbf{x})}, \overline{d'^2(\mathbf{x})})$

$$c(\mathbf{x},t) = \overline{c(\mathbf{x},t)} + c'(\mathbf{x},t) \qquad \sigma^2 = Var[c(\mathbf{x},t)] = \overline{c^2(\mathbf{x},t)} - \overline{c(\mathbf{x},t)}^2 = \overline{c'^2(\mathbf{x},t)}$$

VTHREAT **HPAC**



Individual Plume Realization — **Temporally Averaged Ensemble Average** — **Ensemble-Averaged Plume**

Haber's Law

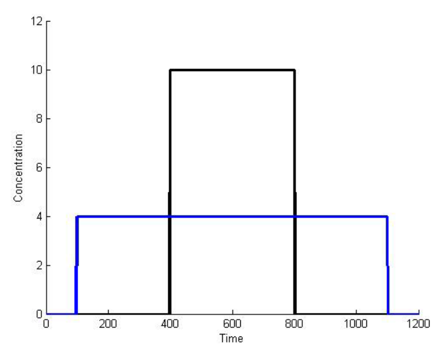
- Most AT&D models calculate toxic effects as a function of only the total dosage of the exposure (Haber's Law).
  - Haber's Law relationships are established empirically for dosages based on constant-concentration exposures:

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

  - 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.



IDA | Toxic Load Model

- 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"

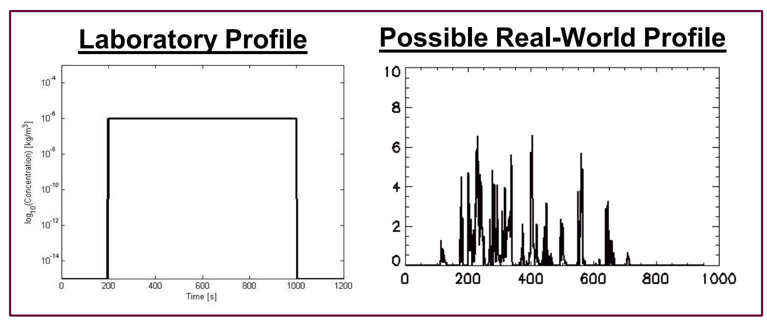
$$TL(\mathbf{x}) = (C(\mathbf{x}))^n T$$

  - *n* is the "toxic load exponent," a chemical-dependent parameter determined from exposure-response data
  - The toxic load model is experimentally verified only for constant-concentration exposures

- For $n > 1$, high-concentration short-duration exposures will produce a stronger toxic effect than low-concentration long-duration exposures.

- Many extensions of this toxic load model have been proposed for time-dependent exposures including ten Berge

$$TL_{TB}(x) = \int c^n(\tau)d\tau = \sum_{i=0}^{K} c^n(x,t_k)\Delta t$$



3

Intuitive Way to do CA based on Dosages

- For T&D models that only output ensemble-mean concentration/dosage and CA based on Dosages

$$x \rightarrow \overline{c}(t,x) \rightarrow \overline{D}(x) \rightarrow Cas(\overline{D}(x)) \neq \overline{Cas(D(x))}$$

Extension to different spatial locations could be used for hazard area assessment (e.g., area above specified threshold)

Extension to different spatial locations could be used to estimate total casualties

This quantity plus an estimate of the variance is actually desired by users for CA

In addition to expected values (e.g., hazard area or casualties), user might be interested in variances

IDA | Dosage Based CA in HPAC

- Question: What kind of dosage based consequence assessment could be calculated in HPAC? How do they compare with each other for a military relevant small chemical attack scenario?

- Given a prescribed threshold level *l* and exposure *d*, let

$$A(d,l) = \begin{cases} 1 & \text{if } d > l \\ 0 & \text{otherwise} \end{cases}$$

- Then, given an exposure function *E* defined at all spatial locations **x**, define area within contour (or hazard area as) as

$$Area(E,l) = \int_{\mathbf{x}} A(E(\mathbf{x}),l)\,d\mathbf{x}$$

Dosage Based CA in HPAC:
Prescribed threshold level *l*, *LCt_{50}* and probit *b*

- Method 1 based on ensemble-averaged dosage

$$Area(\bar{d}) = \int_{\mathbf{x}} A(\bar{d}_{\mathbf{x}}, l)\,d\mathbf{x} \qquad Cas(\bar{d}) = \int_{\mathbf{x}} \Phi\left(b \log_{10}\left(\frac{\bar{d}_{\mathbf{x}}}{LCt_{50}}\right)\right) d\mathbf{x}$$

- Method 2 utilizes ensemble-averaged dosage, dosage variance and assumption that dosages are distributed according to clip-normal distribution $p_{CN}(\tau;\mu_{\mathbf{x}},\sigma_{\mathbf{x}})$
  - For hazard area calculation

$$E[A(\bullet,l)] = \int_0^\infty A(\tau,l)\,p(\tau;\mu_{\mathbf{x}},\sigma_{\mathbf{x}})\,d\tau = \int_l^\infty p_{CN}(\tau;\mu_{\mathbf{x}},\sigma_{\mathbf{x}})\,d\tau = \int_l^\infty N(\tau;\mu_{\mathbf{x}},\sigma_{\mathbf{x}})\,d\tau$$

$$E[A(\bullet,l)] = 1 - \Phi(l;\mu_{\mathbf{x}},\sigma_{\mathbf{x}}) = \frac{1}{2}\left[1 - erf\left(\frac{l-\mu_{\mathbf{x}}}{\sigma_{\mathbf{x}}\sqrt{2}}\right)\right] \qquad \overline{Area\,(l)} = \frac{1}{2}\int_{\mathbf{x}}\left[1 - erf\left(\frac{l-\mu_{\mathbf{x}}}{\sigma_{\mathbf{x}}\sqrt{2}}\right)\right] d\mathbf{x}$$

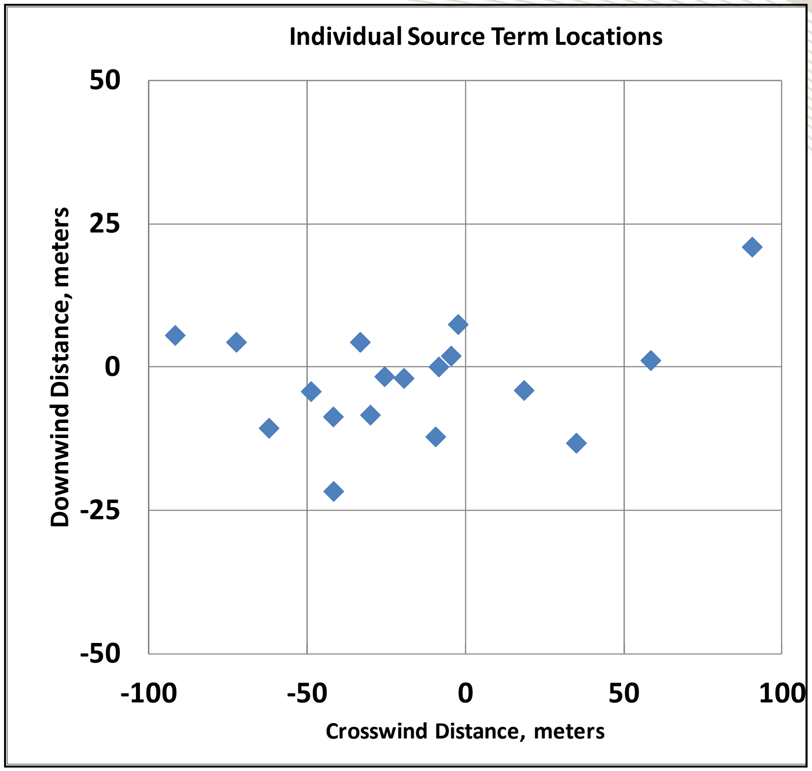
  - Casualties calculation requires numerical integration

$$\overline{Cas} = \int_{\mathbf{x}}\int_0^\infty Cas(\tau)\,p_{CN}(\tau;\mu_{\mathbf{x}},\sigma_{\mathbf{x}})\,d\tau\,d\mathbf{x} = \int_{\mathbf{x}}\int_0^\infty \Phi\left(b\log_{10}\left(\frac{\tau}{LCt_{50}}\right)\right) p_{CN}(\tau;\mu_{\mathbf{x}},\sigma_{\mathbf{x}})\,d\tau$$

For casualty assessment assume uniform population density set to unity
$\mu_{\mathbf{x}}$ and $\sigma_{\mathbf{x}}$ are obtained from d and d'^2 by numerical inversion of a somewhat complicated equation
$\Phi(\bullet)$ denotes cumulative density function for standard normal distribution
$\Phi(\bullet;\mu,\sigma)$ denotes cumulative density function for normal distribution with mean μ and standard deviation σ

IDA | Small Scale Chemical Attack Parameters

- 18 artillery shells (155mm)
  - Each containing 1.6kg Sarin
- Target zone: 200m x 100m
- Terrain: Urban
- Meteorological conditions:
  - 5, 10, & 15km/hr. winds
  - Moderately Stable (PG6) or Slightly Unstable (PG3) atmosphere
- Population density is assumed to be uniform



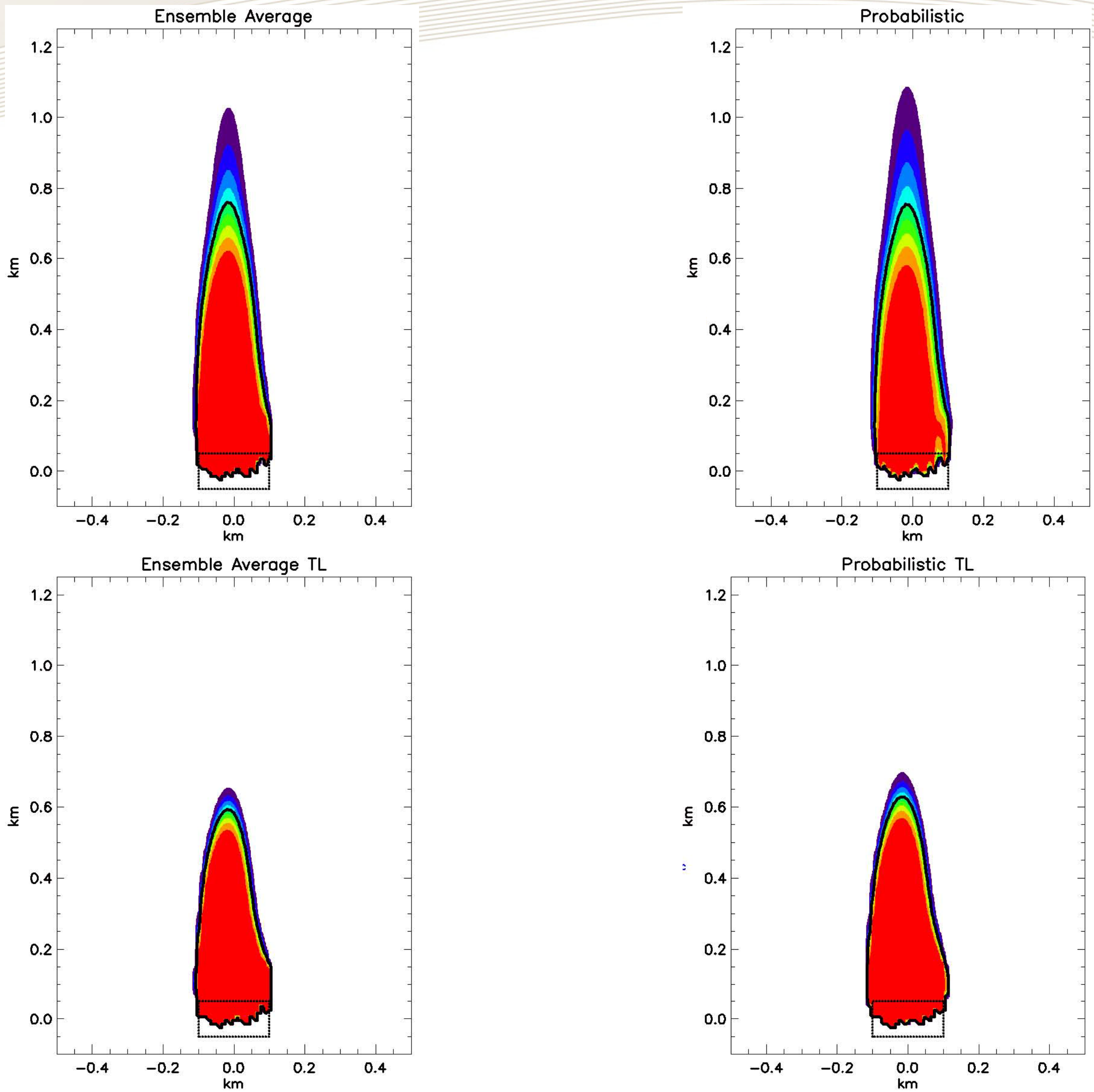
- Two potential analysis areas of Interest for CA
  - On-target hazard area/casualties
  - Full extent of hazard area/casualties

Casualty Calculations Based on Dosage and Toxic Load Model

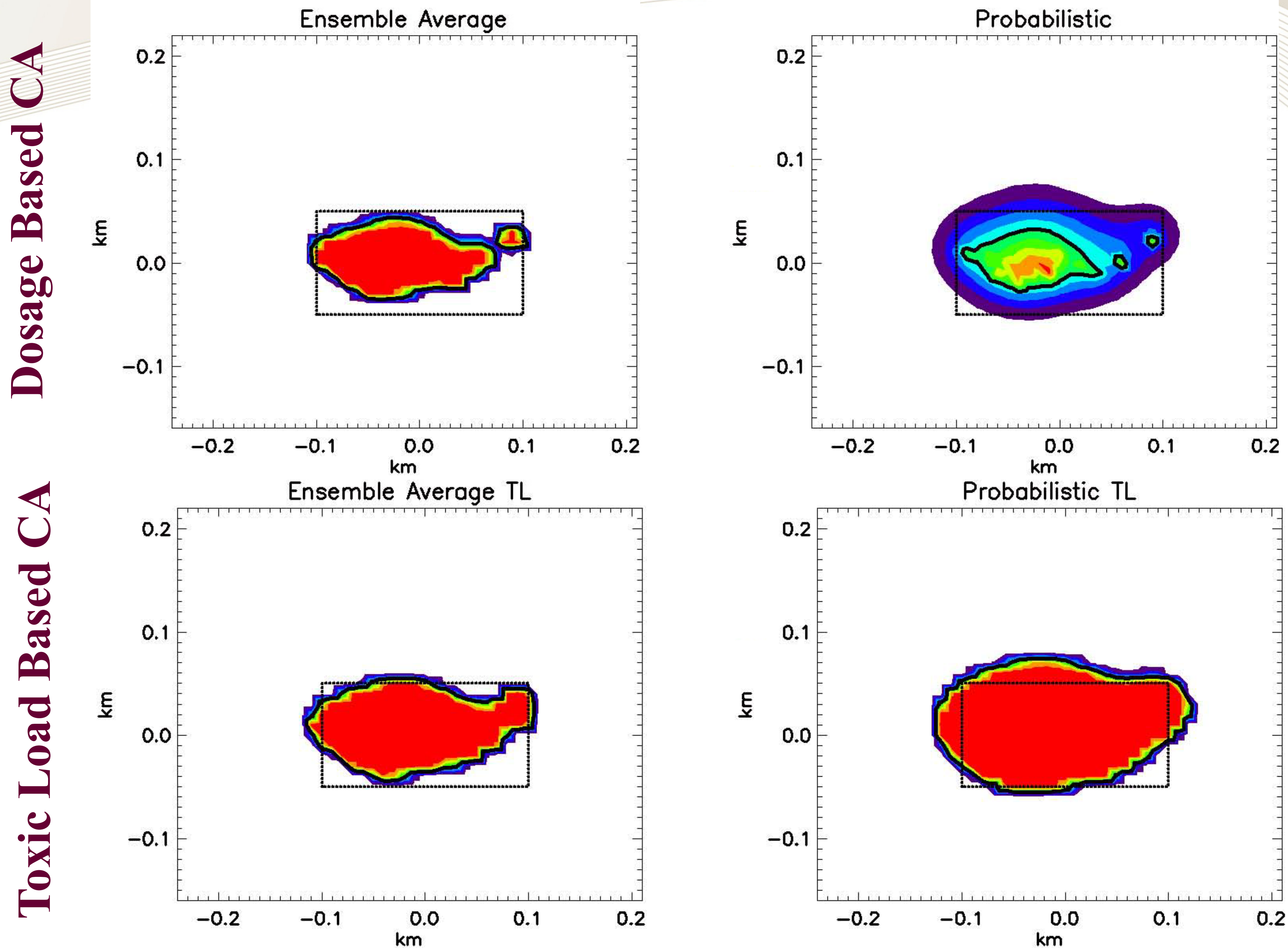
Typical Casualties Contours for Moderately Stable Atmosphere (PG=6, Wind Speed = 10 km/hr)

Dosage Based CA

Toxic Load Based CA

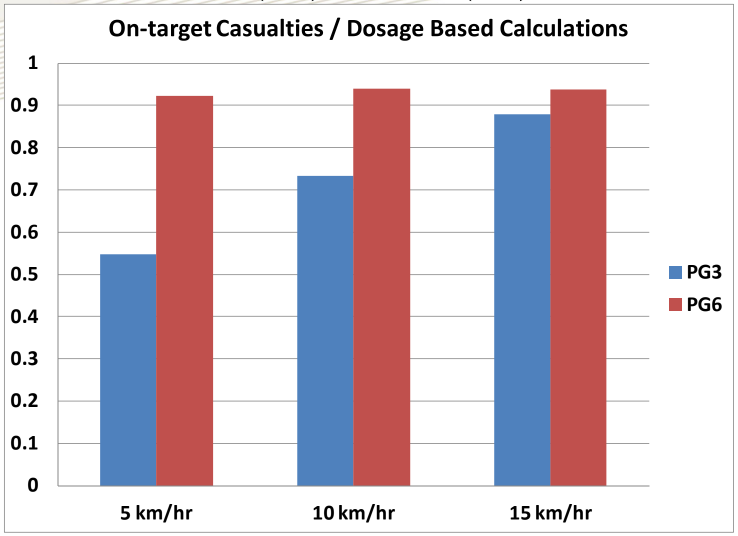


Typical Casualties Contours for Slightly Unstable Atmosphere (PG=3, Wind Speed = 10 km/hr)

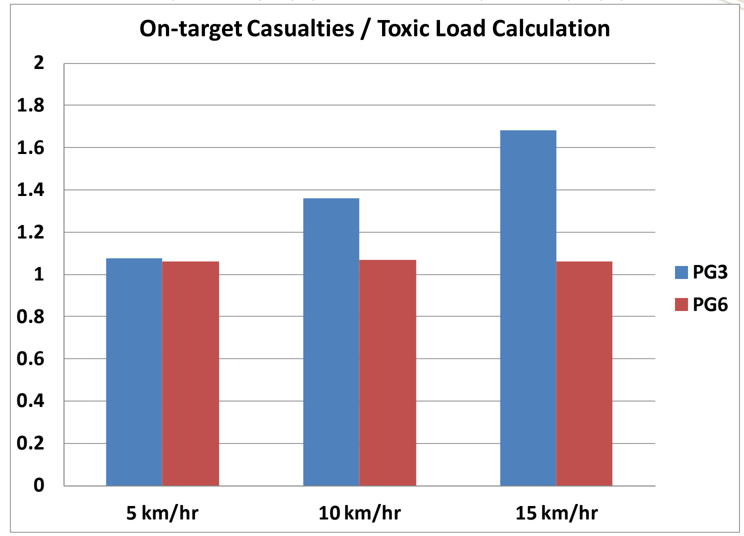


Results for Casualties / On-Target Attack

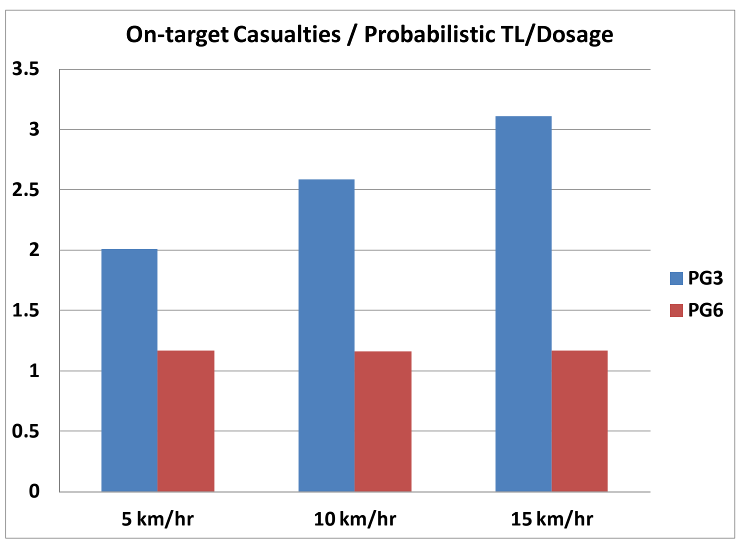
$$\overline{Cas(D)} / Cas(\overline{D})$$



$$Cas(\overline{TL(c)}) / Cas(TL(\bar{c}))$$

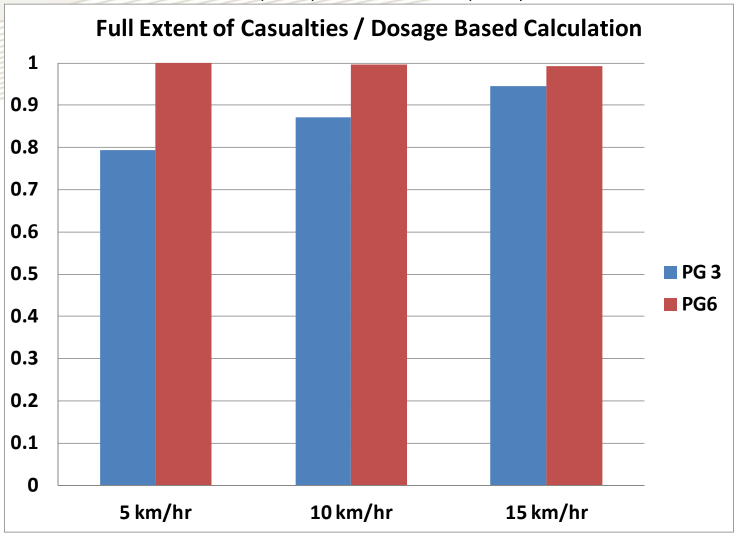


$$Cas(\overline{TL(c)}) / \overline{Cas(D)}$$

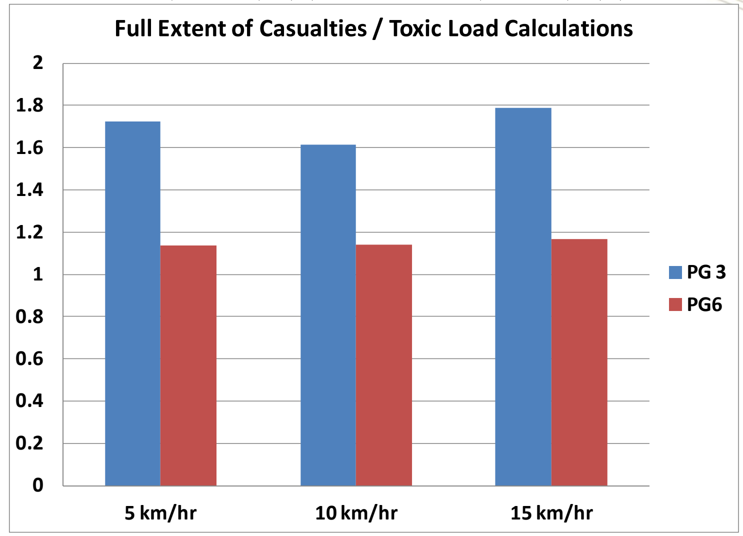


Results for Casualties / Full extent of the plume

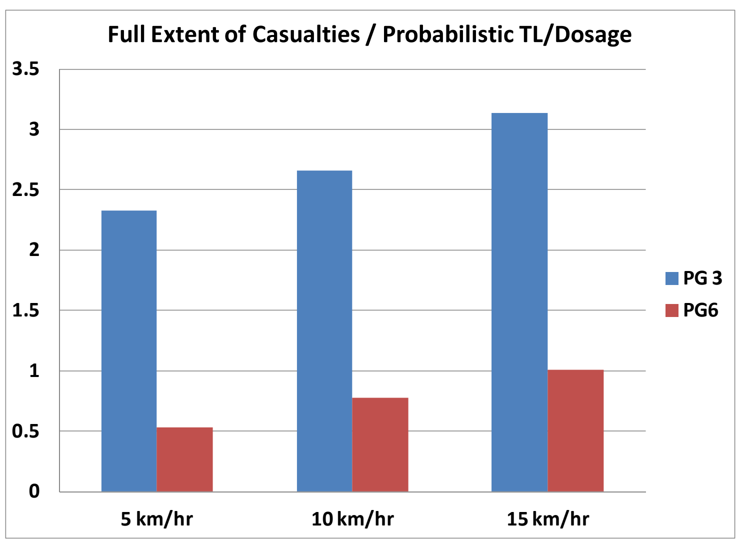
$$\overline{Cas(D)} / Cas(\overline{D})$$



$$Cas(\overline{TL(c)}) / Cas(TL(\overline{c}))$$

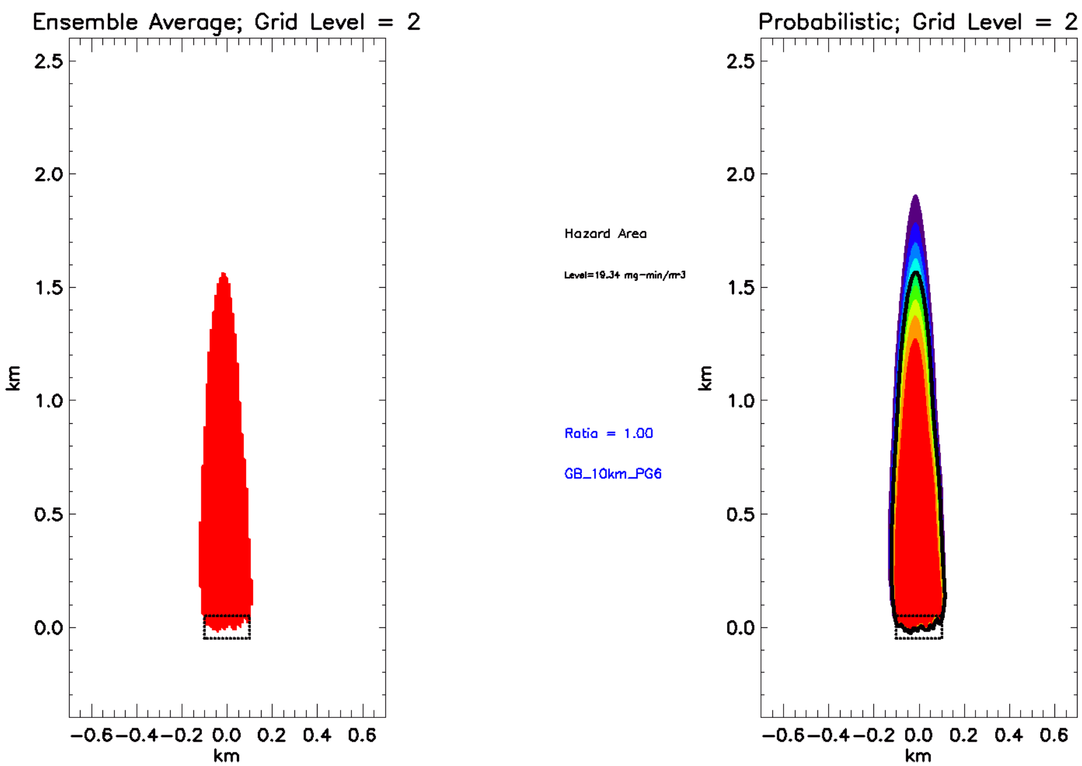


$$Cas(\overline{TL(c)}) / \overline{Cas(D)}$$

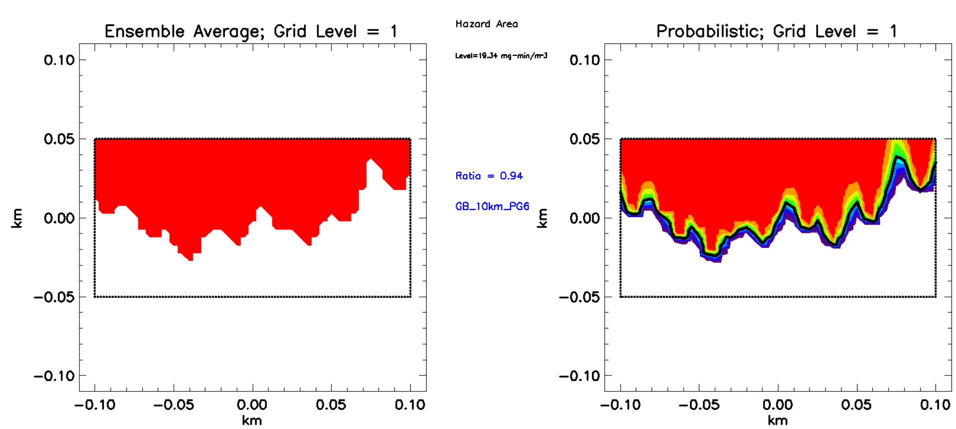


Hazard Area Calculations Based on Dosages

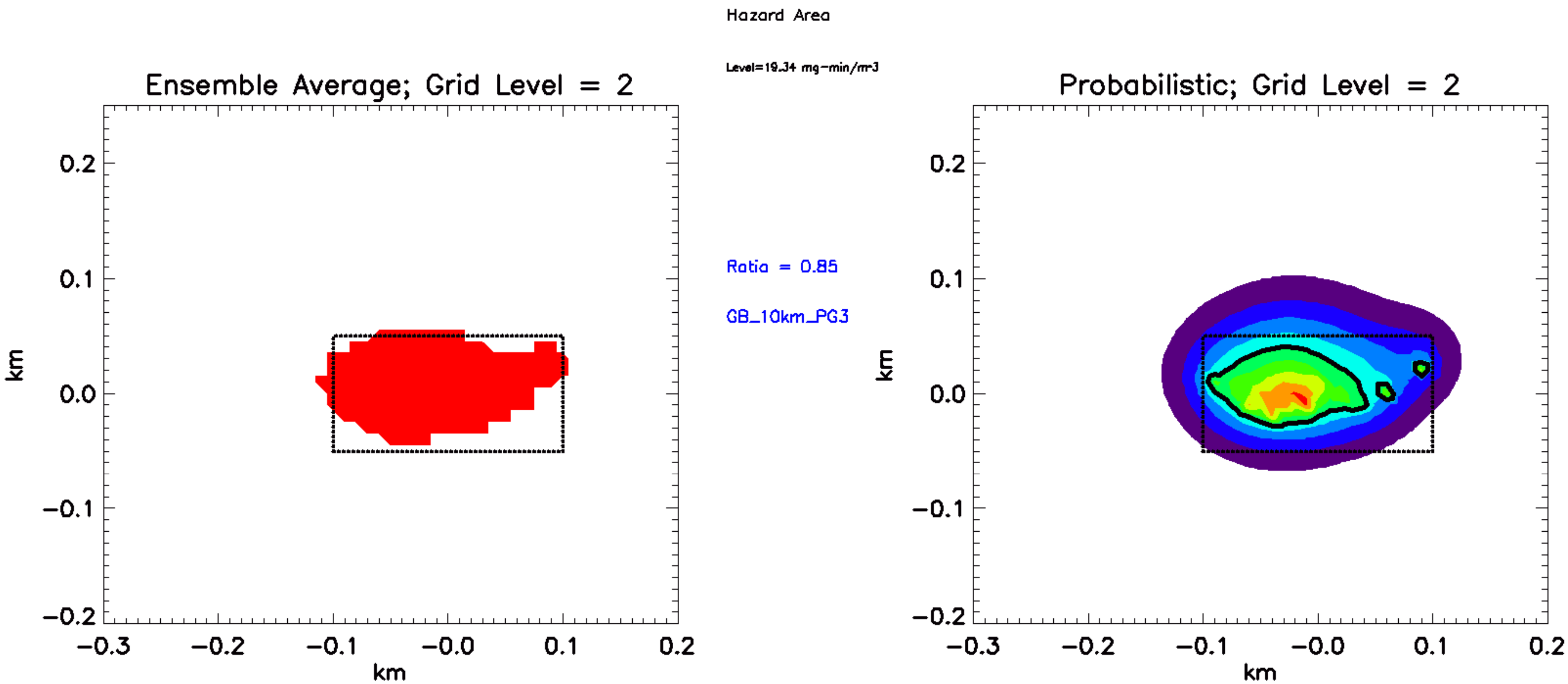
Typical Hazard Area Contours (PG=6) / Hazard Level = $LCt_{0.1}$



On-target Attack

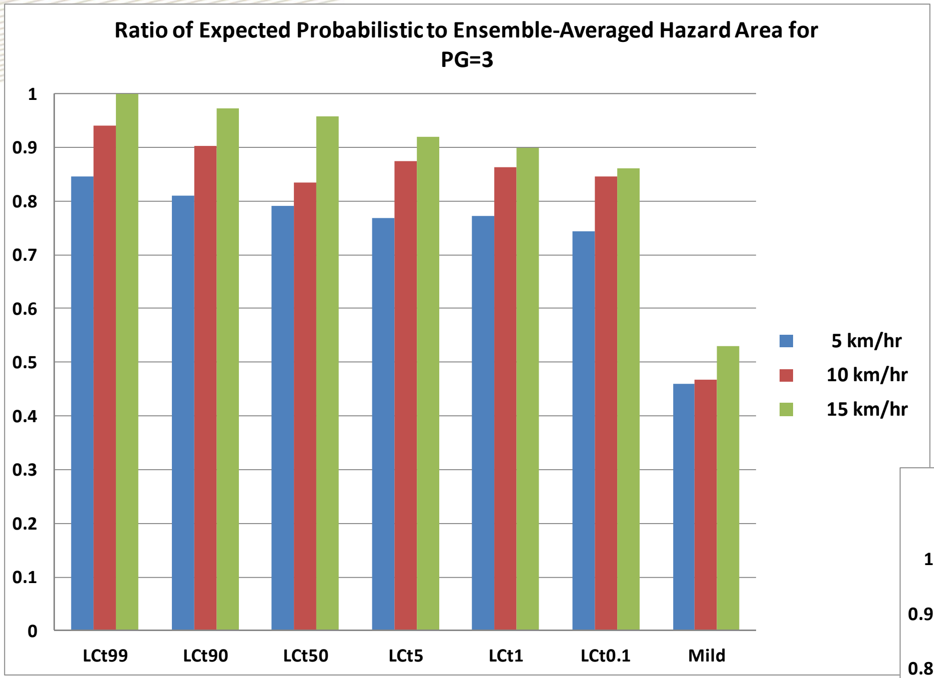


Typical Hazard Area Contours (PG=3) / Hazard Level = $LCt_{0.1}$

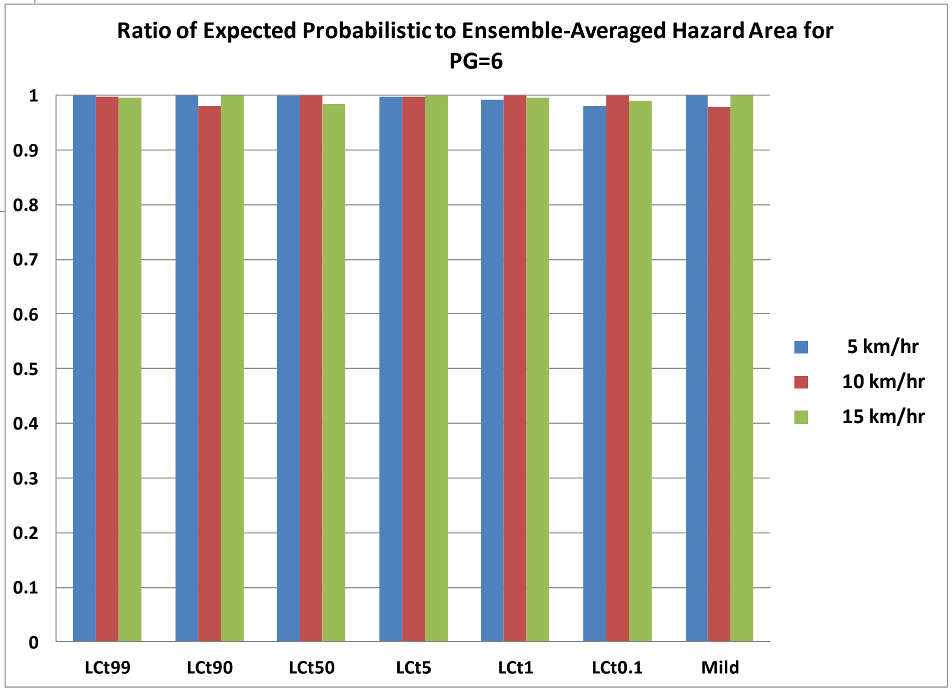


Result for Hazard Area Calculations / Full Extent

Slightly Unstable Atmosphere

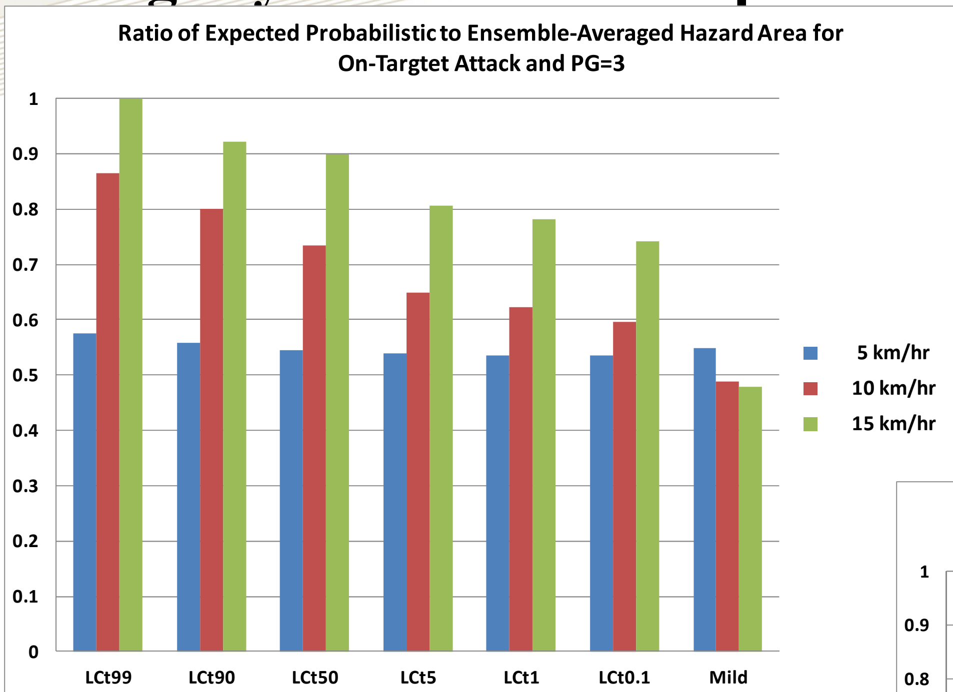


Moderately Stable Atmosphere

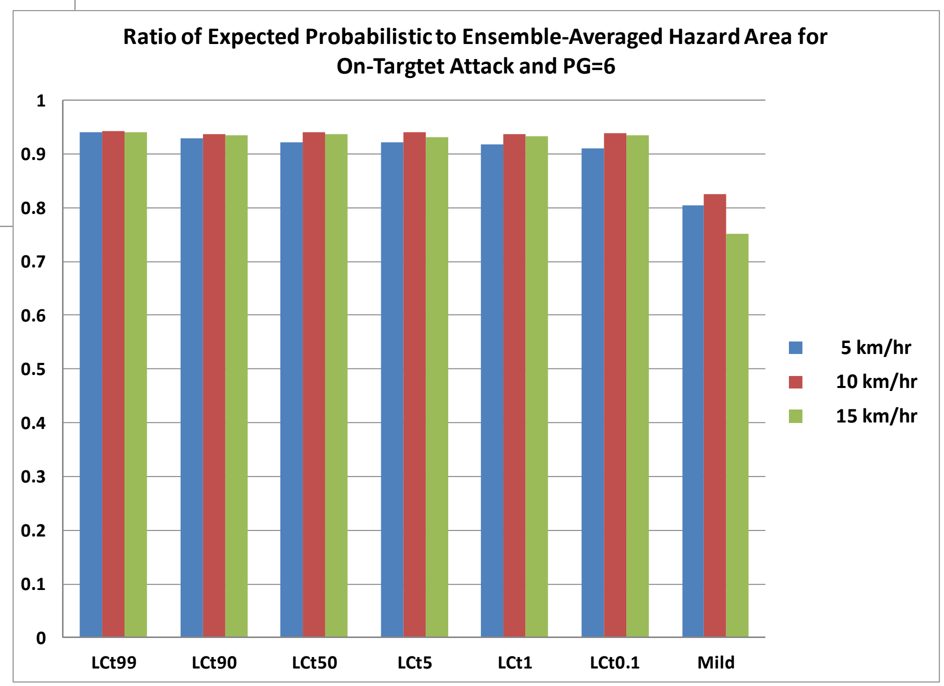


IDA | Result for Hazard Area Calculations / On-Target

Slightly Unstable Atmosphere



Moderately Stable Atmosphere



IDA

Summary

- Some care should be exercised when using HPAC for both dosage and toxic load based consequence assessment
  - Two methods to do CA within HPAC/JEM
    - Based on ensemble-averaged dosage or concentration + toxic load
    - Based on full probabilistic dosage/toxic load exposure utilizing ensemble-averaged dosage/concentration, variance and assumption of a clip-normal distribution
- For single small scale chemical attack and limited parametric variations (e.g., three wind speeds and two atmospheric stability categories) considered here
  - Moderately stable atmospheric conditions yields comparable consequence assessments using ensemble-averaged and probabilistic methodology for either dosage or toxic load based CA
    - However, Haber's law and toxic load model casualties could differ by a factor of two when full extent of the plume is considered
    - Dosage based hazardous plume have a longer downwind spatial extent than toxic load based hazardous plume
  - Slightly unstable atmospheric condition results in significant variations in CA depending on type of toxicity model used (e.g., dosage or toxic load)
    - For dosage based toxicity model
      - Depending on wind speed and size of the target area, ***over-prediction*** up to a factor of two is possible
      - Spatial distribution of casualties and hazard could be significantly different between two methods of doing CA
    - For toxic load model
      - Depending on wind speed and size of the target area, ***under-prediction*** up to 60-80% is possible
    - Toxic load model casualties could be a factor of 3 higher than casualties based on Haber's law

BACKUPS

IDA Toxic Load Based Consequence Assessment

- Toxic Load based CA are non-trivial as the math is more difficult:

$$x(t) \rightarrow \overline{c(t,x)} \rightarrow \overline{TL(c(t,x))} \rightarrow Cas(\overline{TL(c(t,x))}) \neq \overline{Cas(TL(c(t,x)))}$$

This step can be done when distribution of concentration fluctuations is assumed (e.g., SCIPUFF)

This step cannot be done with SCIPUFF without additional assumption of distribution of toxic load exposures

HPAC Based Calculations of Toxic Load Exposure

- Method 1 uses ensemble-averaged concentration $\overline{c(\mathbf{x},t)}$ alone

$$TL_{.}(\overline{c(\mathbf{x})}) = \sum_{k=1}^{K} \overline{c(\mathbf{x},t_k)}^{\,n} \Delta t$$

Here $\overline{c(\mathbf{x},t_k)}$ denote ensemble-average concentration at time t_k

- Method 2 uses both ensemble-averaged concentration and concentration variance to numerically calculate ensemble-averaged toxic load

$$\overline{TL(c(\mathbf{x}))} = \frac{1}{M}\sum_{m=1}^{M} TL(c_m(\mathbf{x})) = \frac{1}{M}\sum_{m=1}^{M}\sum_{k=1}^{K} c_m^n(\mathbf{x},t_k)\Delta t =$$

$$= \sum_{k=1}^{K}\left(\frac{1}{M}\sum_{m=1}^{M} c_m^n(\mathbf{x},t_k)\right)\Delta t = \sum_{k=1}^{K} \overline{c^n(\mathbf{x},t_k)}\Delta t$$

$$\overline{c^n(\mathbf{x},t_k)} = \int_0^\infty s^n p_{CN}(s)ds = \int_0^\infty s^n \frac{1}{\sigma_k(\mathbf{x})\sqrt{2\pi}} \exp\left(-\frac{(s-\mu_k(\mathbf{x}))^2}{2\sigma_k^2(\mathbf{x})}\right)ds$$

- Noting that function $f(r) = r^n$ is a convex function for *n*>1, we arrive

$$\overline{c(\mathbf{x},t_k)}^{\,n} \le \overline{c^n(\mathbf{x},t_k)} \quad \text{when } n > 1$$

$$TL_{.}(\overline{c(\mathbf{x})}) \le \overline{TL(c(\mathbf{x}))} \quad \text{when } n > 1$$

μ_k and σ_k are obtained from $\overline{c(\mathbf{x},t_k)}$ and $\overline{c'^2(\mathbf{x},t_k)}$ by numerical inversion of a somewhat "complicated" equation

21

Relationship Between Clip-Normal Distribution and Normal Distribution (as defined by HPAC)

Clip-Normal Distribution

$$p_{CN}(c) = \frac{1}{2}\left(1 - erf\left(\frac{\mu_G}{\sigma_G\sqrt{2}}\right)\right)\delta(c-0) + \frac{1}{\sigma_G\sqrt{2\pi}}\exp\left(-\frac{(c-\mu_G)^2}{2\sigma_G^2}\right), \quad c \geq 0$$

Mean and Sigma of Clip-Normal Distribution

$$\mu = \frac{\sigma_G}{\sqrt{2\pi}}\exp\left(-\frac{\mu_G^2}{2\sigma_G^2}\right) + \frac{\mu_G}{2}\left(1 + erf\left(\frac{\mu_G}{\sigma_G\sqrt{2}}\right)\right)$$

$$\sigma^2 = -\mu^2 + \frac{\sigma_G^2}{2}\left(1 + erf\left(\frac{\mu_G}{\sigma_G\sqrt{2}}\right)\right) + \mu_G\mu$$