Bulk Chemical Source Term Accuracy Requirements

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Good morning/afternoon. I'm … from MEVATEC Corporation. My co-author is …, and our sponsor is Dr. Charles Lind of the Missile Defense Agency. The subject of our presentation is bulk chemical warhead source term accuracy requirements.

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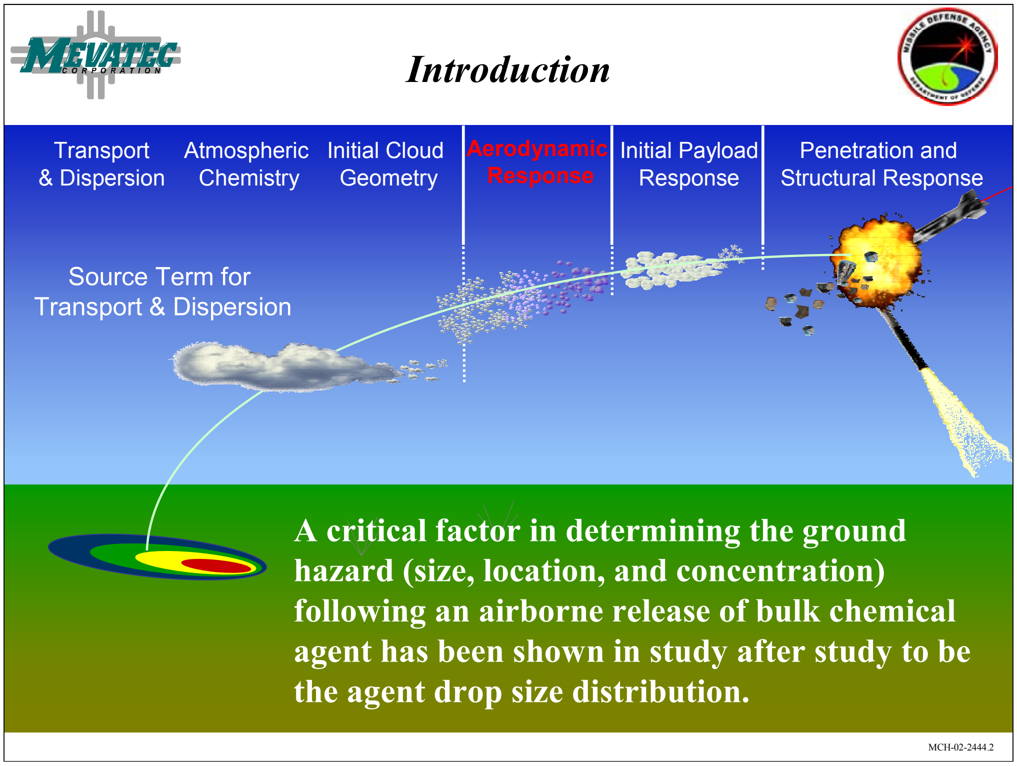
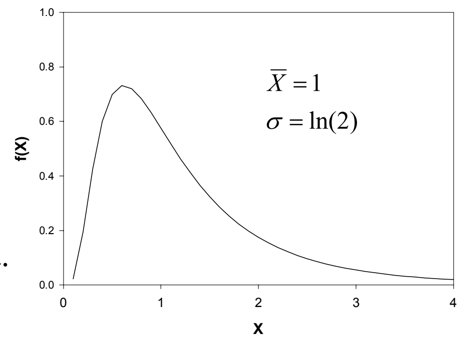


Among the many uncertainties involved in a ground hazard prediction for a bulk chemical release, the agent drop size has been shown in study after study has shown to be of critical importance. Accordingly, the Missile Defense Agency has devoted significant resources seeking an understanding of the drop sizes that would result from an intercept-induced release. Our study is a continuation of that general effort.

Background

- Transport codes (HPAC and VLSTRACK) usually assume a **lognormal** drop size distribution.
- Two-parameter characterization
  - Mass Median Diameter
  - Geometric Sigma
- Current model for MMD is the **Soltisz** algorithm with fixed sigma (1.8).
  - Fit to legacy witness card data.
  - f(agent, speed, altitude)

$$f(X) = \frac{1}{\sqrt{2\pi}\sigma X}\exp\left[-\left(\frac{\ln(X)-\ln(\overline{X})}{2\sigma}\right)^2\right]$$



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Traditionally, chemical weapons effects analyses have assumed a lognormal agent drop size distribution. Used widely within the weapons effects sciences, the lognormal distribution is a relatively simple mathematical expression fully defined by only two numerical parameters: in essence, a mean and a standard deviation, or, in the proper terminology, a droplet Mass Median Diameter (MMD) and a geometric sigma. It has until recently appeared to describe adequately the drop sizes observed from legacy test results, and the method used in MDA's Post-Engagement Ground Effects Model called upon the Soltisz model to predict the MMDA as a function of agent characteristics, reentry speed, and release altitude.

Background (con't)

- Physics-based drop size distribution models are under development. Premier is SAIC's **CASCADE** model.
  - CASCADE distributions are not lognormal and do not conform to any simple analytical description. Each event may result in a **uniquely** shaped distribution.
  - High quality validation data are still missing, including the parent source terms (seed droplet size distribution).
  - There is a significant calculation burden.
- *Just how accurately does one have to know the bulk chemical source term in order to have a confident ground hazard prediction?*

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Part of MDA's effort to understanding the bulk chemical droplet aerodynamic breakup process in the high-speed high-altitude regimes not easily tested has been to develop physics-based models, principally the CASCADE model. The resulting drop size distributions are not lognormal and do not conform to any simple analytical description. The jury is still out on validation of the model, due to a lack of experimental data and some uncertainty regarding the parent source terms used to seed the CASCADE breakup model. But it is clear from studies thus far that the model carries a substantial burden of calculations, adding to the run time for a prediction.

The question that we seek to address here is whether the numerically-intensive details of the distributions yielded by CASCADE make a significant difference to the ground hazard resulting from the chemical agent release, or a simpler approach might suffice.

Parametric Study

- Examine ground effects from a thickened VX bulk chemical release. Vary altitude, reentry speed, and wind conditions.
- Three drop size distribution methods:
  - Lognormal, MMD using the **Soltisz** model, fixed sigma
  - **CASCADE** distribution (physics-based model, unique shape)
  - Lognormal, using **CASCADE MMD** and pseudo sigma calculated from the CASCADE distribution.

Competing models, different MMD

Same MMD, different distribution shapes

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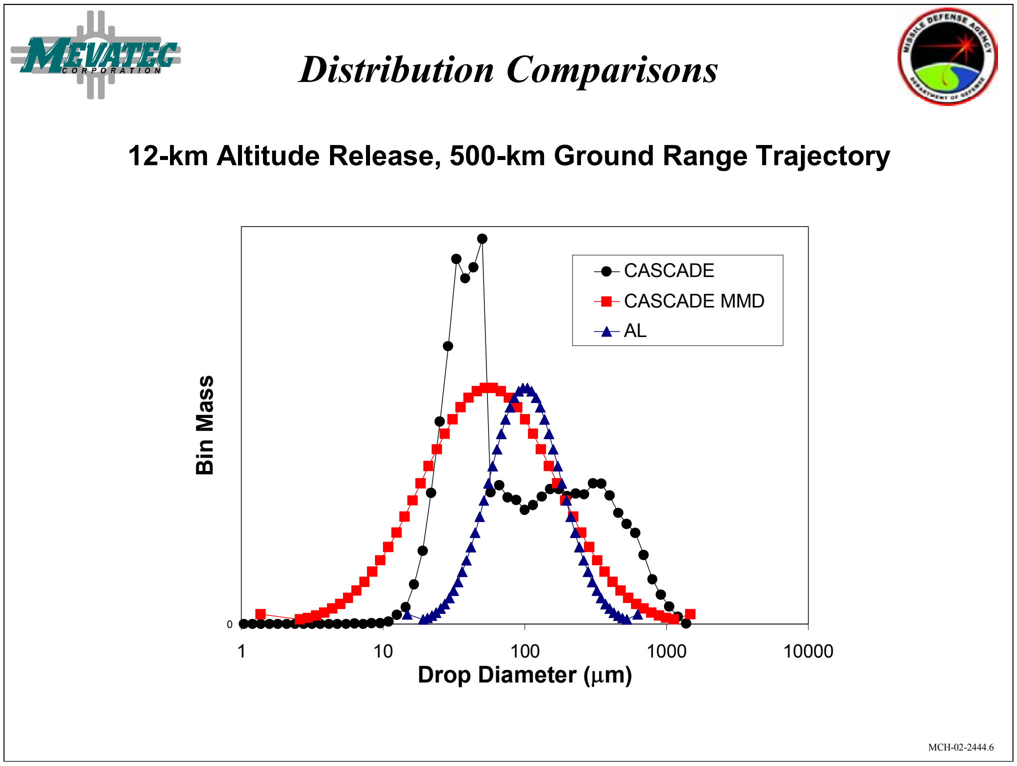
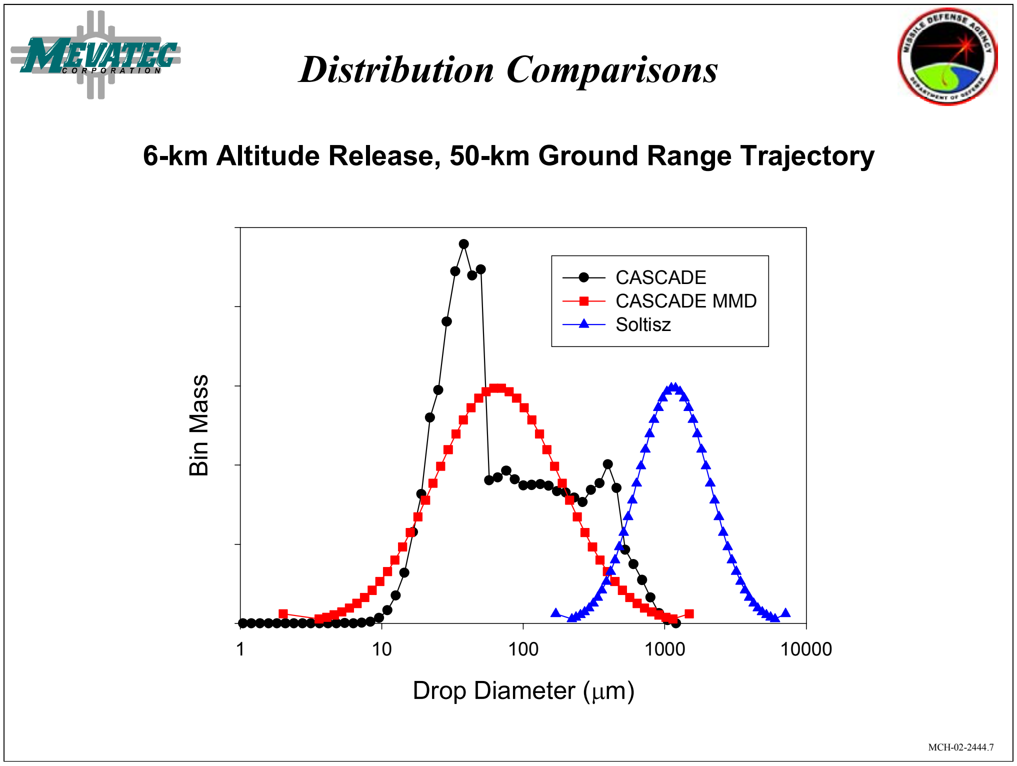
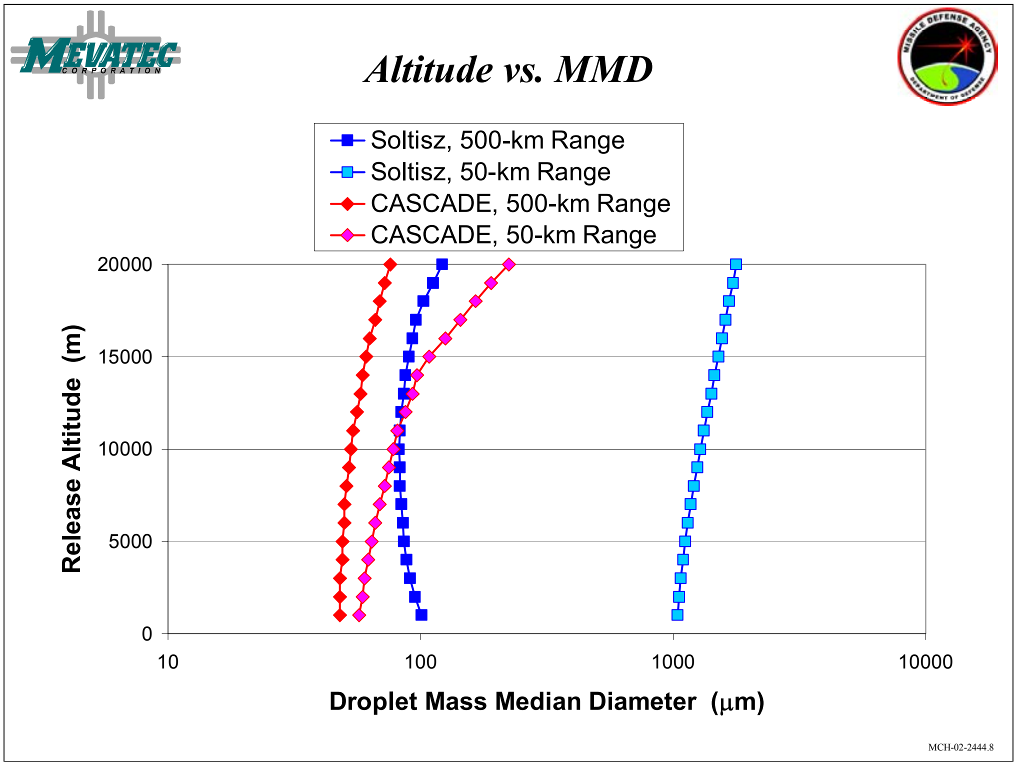
Our approach is to perform a parametric analysis of ground effects resulting from a release of thickened VX at various conditions of release altitude, reentry speed and wind conditions, and utilizing three different methods to determine the droplet size distribution. The first method is to use the traditional lognormal distribution, using the traditional Soltisz model to determine the MMD. The second method is to use the new CASCADE model to develop a detailed droplet size distribution based on the physics of the aerodynamic breakup processes. The third method is to use again a lognormal distribution, but now one intended to match as closely as practical the CASCADE distribution: using the same MMD and a sigma yielding the same maximum droplet size as from CASCADE. Comparing the Soltisz and CASCADE results will illustrate to some extent how the two competing models differ in their predictions, but as the "best" parent source term for CASCADE has not yet been determined, these comparisons must be viewed exploratory, only. Comparing the CASCADE and CASCADE MMD lognormal distributions will address directly whether the detailed differing shapes of the distributions really matter.



This slide compares the three distributions for a particular set of release conditions: an altitude of 12 km at a reentry speed resulting from a 500-km ground range trajectory. Note that the droplet diameter axis is a log scale, giving the two lognormal distributions the characteristic Gaussian shape. The Soltisz MMD is always greater than the CASCADE MMD for all our release conditions, though the magnitude of the difference varies. Here, with the 500-km range trajectory they differ by only about 50%. Importantly, because the sigma of the CASCADE MMD distribution has been matched to yield the same maximum drop size as the CASCADE distribution, the CASCADE MMD distribution actually has larger drops than the Solitisz. The CASCADE distribution is quite a different shape: a large number of drops just below the MMD, and a plateau of large drops above the MMD before falling off sharply near the maximum surviving drop size. The fraction of large drops is very important for the releases at reasonable intercept altitudes, for there only the largest drops contribute to deposition densities large enough to constitute a casualty hazard. Much of the interpretation of ground effects plots to follow later in this presentation will revolve around this fact.



Here are the three distributions for a release on a much shorter 50-km trajectory, meaning a much slower reentry speed. The CASCADE distribution has not changed a great deal, but the Soltisz MMD has increased substantially. Among these three distributions, the Soltisz clearly has the largest drops and in great numbers.



Here are the MMD's as a function of altitude, resulting from Soltisz (in blue and light blue) and CASCADE (red and pink) for a 500- and a 50-km TBM trajectory. For a given reentry speed and altitude, the Soltisz MMD is always greater than the CASCADE MMD: by over an order of magnitude for the 50-km trajectory (growing with altitude), but by less than a factor of two for the 500-km trajectory.

Study Scenario

- Bulk chemical TBM payload
  - 311 kg thickened VX
  - Entire payload released into the air
- Trajectory from north into Osan Airbase, South Korea
- 1996 winds, Air Force Combat Climatology Center data
  - Single-wind comparisons: 1 Jan 00Z & 1 Jun 00Z
  - Many-wind: one day (00, 06, 12, 18Z) every week
- Casualties calculated using PEGEM 4.1 with VLSTRACK
  - Uniform population density, unprotected, 1 person/hectare
- Hit-To-Kill intercepts at altitudes from 1 to 20 km

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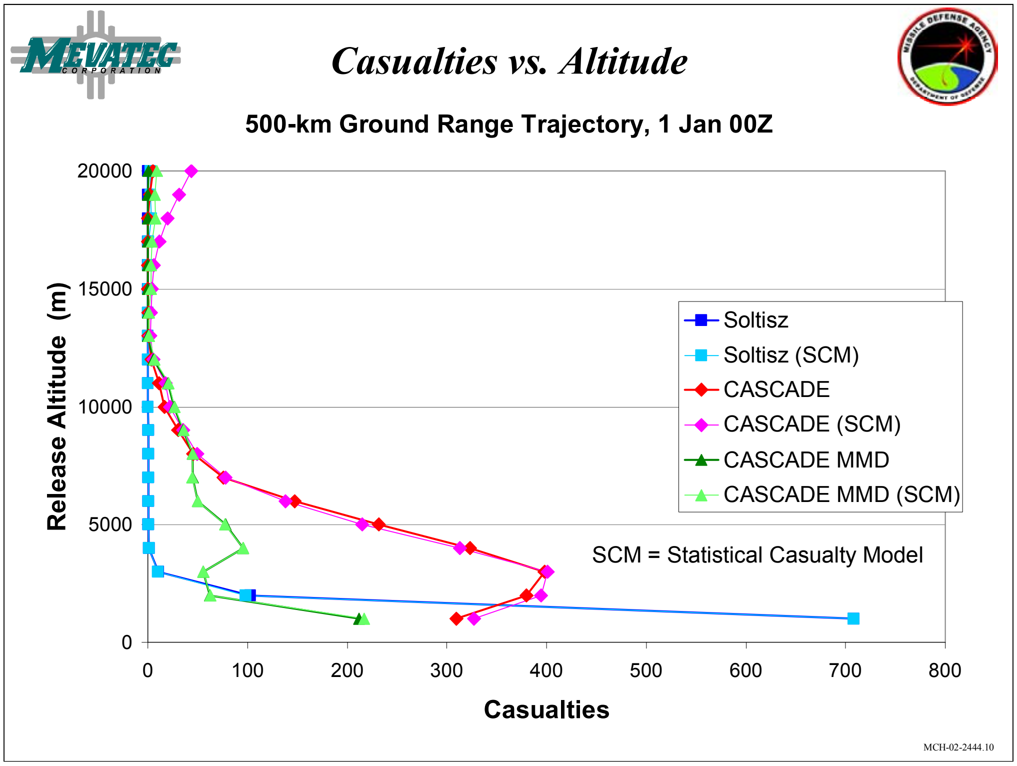
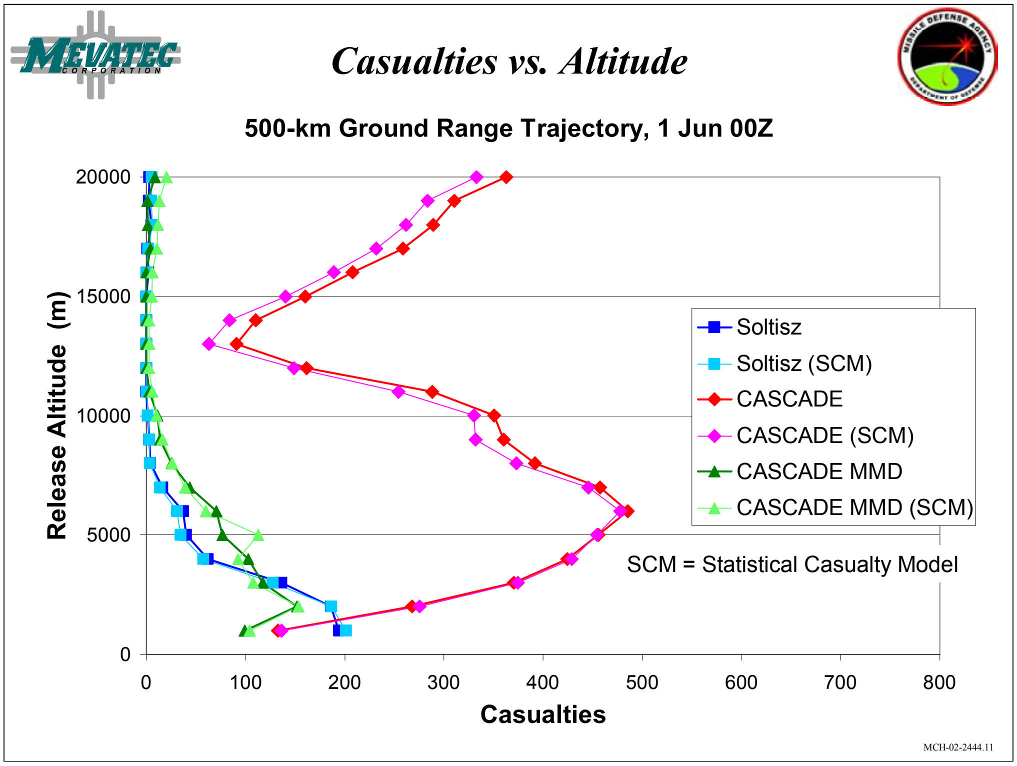
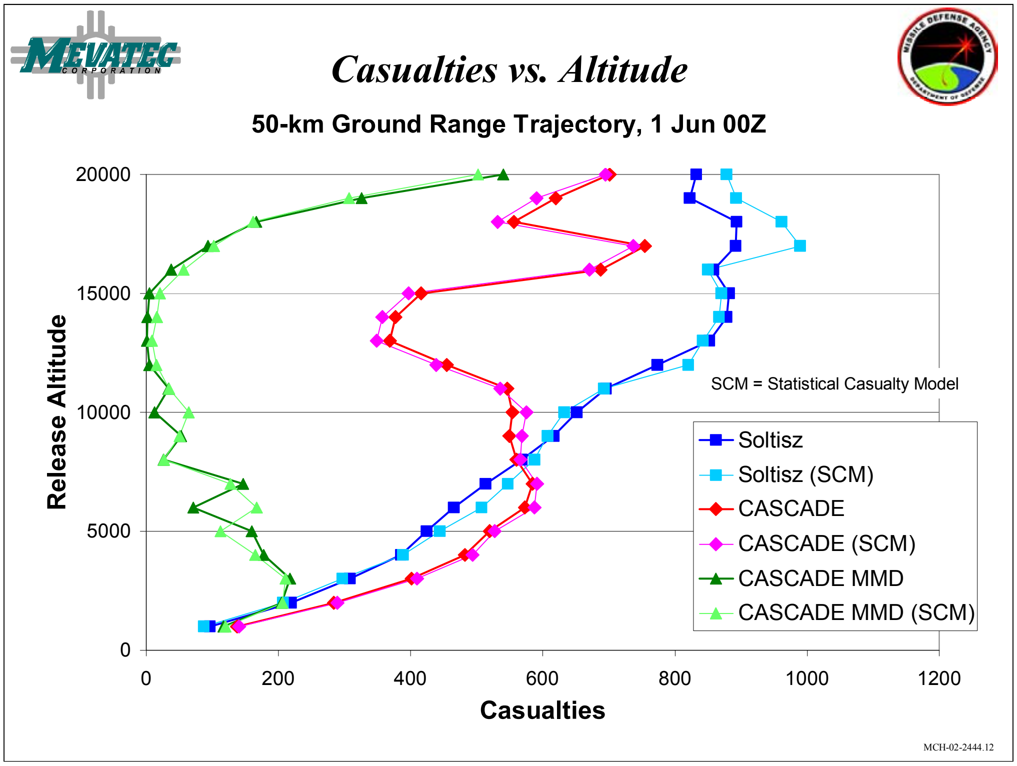
These are the remaining parameters of our study. The threat carries 311 kg of thickened VX toward Osan Airbase. The wind conditions are from 1996. We begin with a close examination of results as a function of altitude for two wind conditions: 1 January and 1 June, both at midnight Zulu time. This will demonstrate clearly that there are significant differences between the three distributions. But one lesson that we have learned well is that one should not jump to draw conclusions from one or two wind conditions. So we also examine the results for a few selected altitudes results for over 200 wind conditions. This will yield a better picture of how widely the predictions vary with droplet size distribution method. The measure of effects will be casualties among a very thin uniform population of 1 person per hectare. We use version 4.1 of the Post-Engagement Ground Effects model with the VLSTRACK transport code. We assume Hit-To-Kill intercepts up to an altitude of 20 km, the current limit for the CASCADE model.



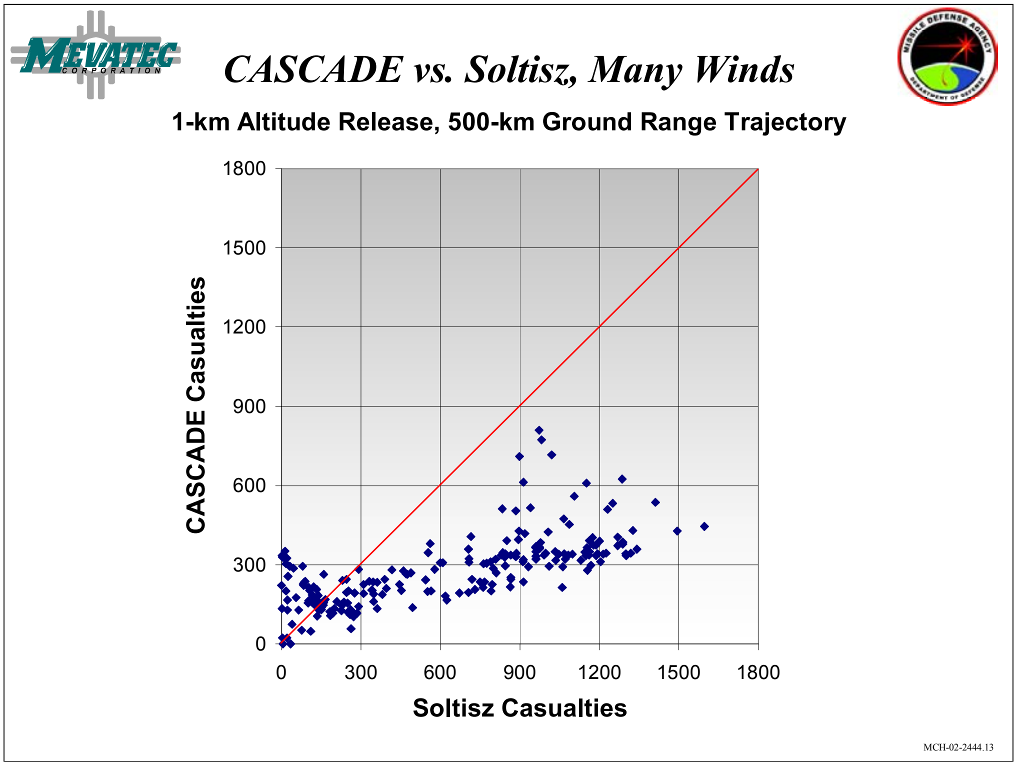
These are results for the three distributions for intercepts along the 500-km trajectory with the winds on 1 January at 00Z. The Soltisz model results are in blue, the CASCADE in red, and the CASCADE MMD in green. The results for the three models are here similar for intercepts above 10 km (at least on this scale), but quite different below. The large drops in the CASCADE distribution are the key ingredient until the very lowest altitudes, where the smaller drop sizes participate in the casualty hazard. The larger sigma of the CASCADE MMD lognormal results in the casualty potential of this model exceeding that of the Soltisz for these release conditions, again because of the presence of the large drops in greater numbers. Another interesting feature of this plot is that it shows the casualty results using PEGEM's "SCM" (Statistical Casualty Model) capability to consider the statistics of the impact of individual large droplets, in addition to the traditional method of treating only a local average agent deposition density. Because we anticipated casualty effects from large drops, we paid the price of lengthy calculations for these initial investigations in order to judge the value of the SCM model. Note that the SCM model has resulted in significant differences for the releases above 16 km, particularly for the CASCADE model.



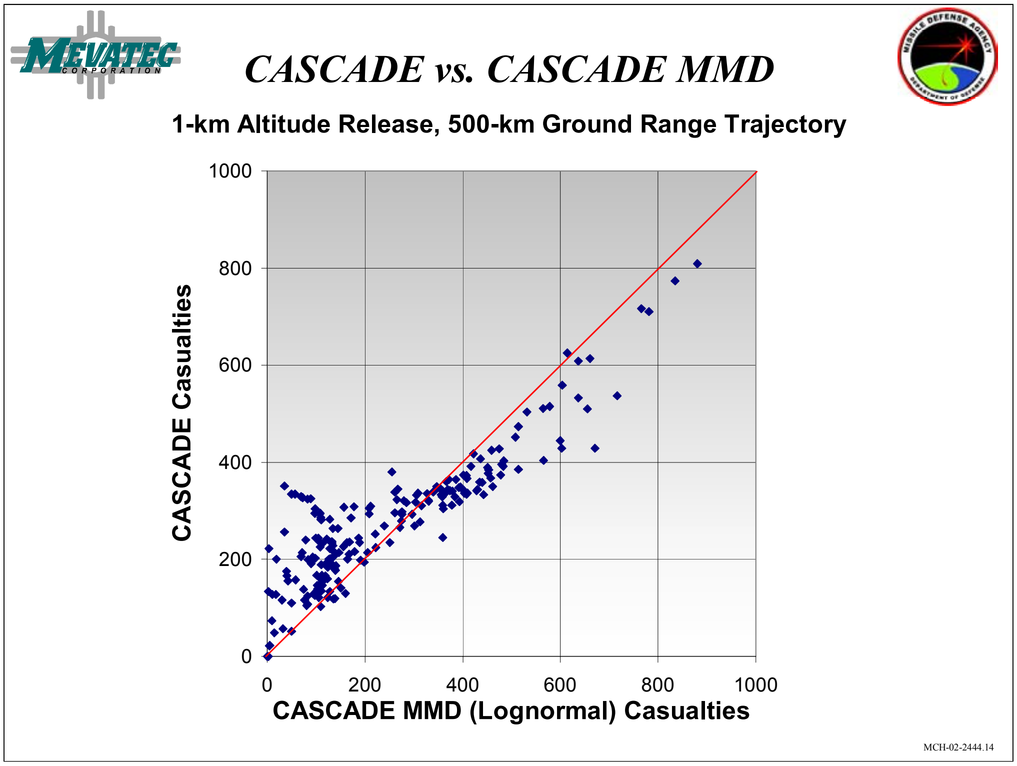
These are the same release conditions, but for the winds on 1 June. The same general trends apply. Above the very lowest release altitudes, the large drops drive the ground hazard: CASCADE has the largest fraction of large drops, followed by CASCADE MMD due to the large lognormal sigma, then Soltisz.



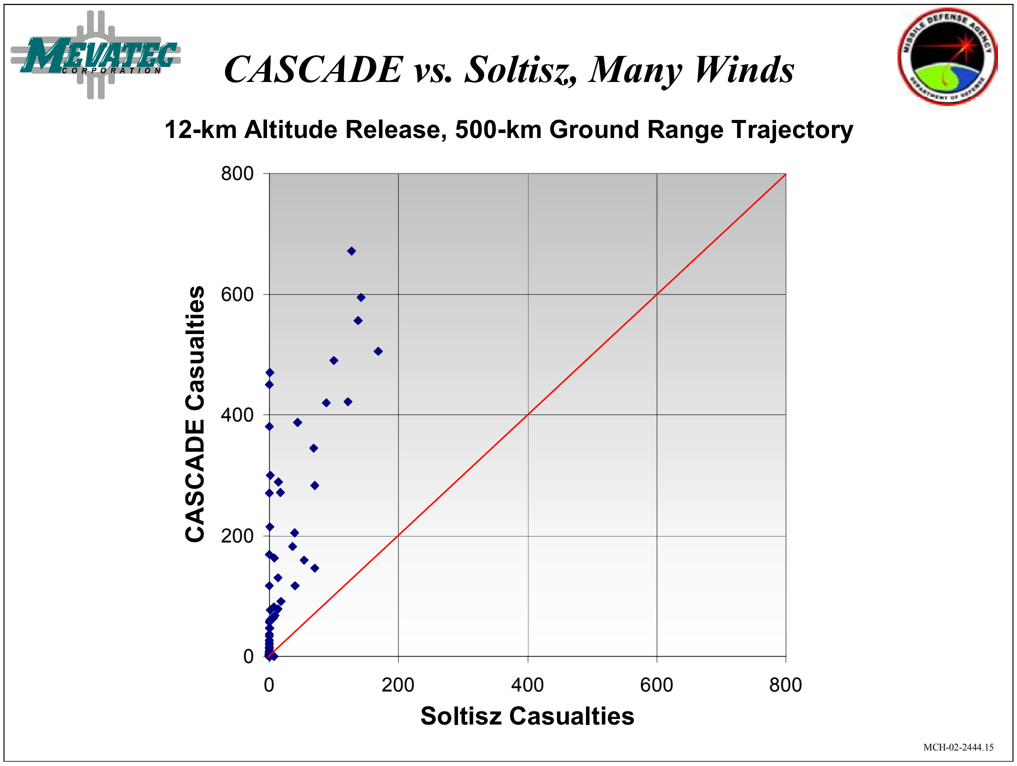
If you're tempted to over generalize those trends, this slide should make you reconsider. The winds are still for 1 June, but now the trajectory has only a 50-km ground range. The CASCADE distribution still has a larger percentage of large drops than the CASCADE MMD lognormal distribution, resulting in a larger number of casualties. Now, however, the Soltisz model is the more pessimistic at the higher altitudes. Recall that with this trajectory the Soltisz MMD is greater than the CASCADE by over an order of magnitude, and the discrepancy grows with altitude.



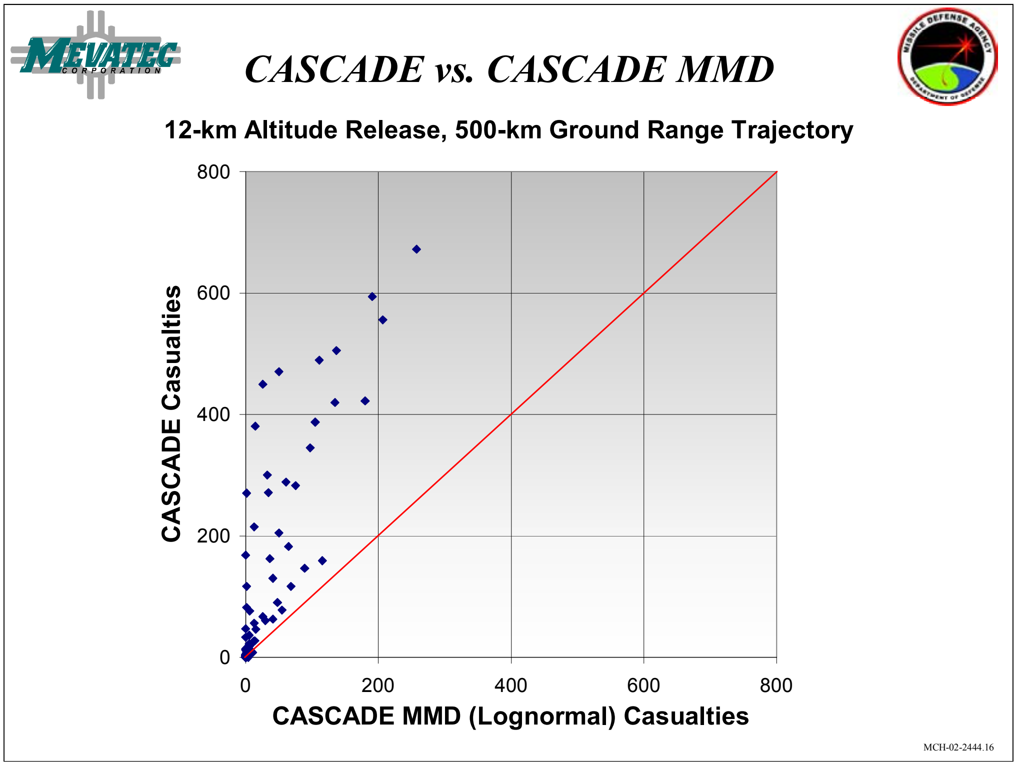
Now we switch to an examination of many winds, narrowing the plot to a single release altitude (in this case 1 km, with the 500-km trajectory), and comparing only two of the droplet size distribution methods (in this case CASCADE and Soltisz). Each blue dot represents a pair of results, from CASCADE and Soltisz, for one of 212 wind conditions. If the two models were predicting exactly the same drop size distributions, each of the blue dots would like along the red line at 45-degrees. At this very low release altitude, Soltisz tends to produce the more casualties, but not always.



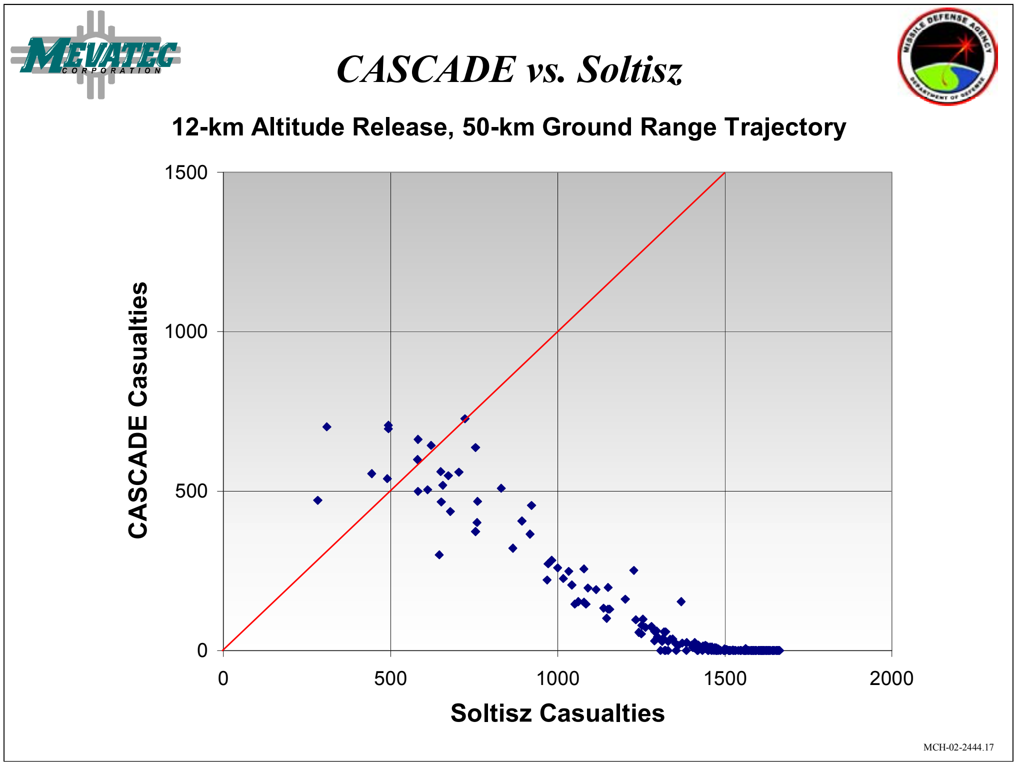
Switching to a comparison of CASCADE with the CASCADE MMD lognormal, we see that these two methods compare favorably under the conditions of 1 km altitude and 500-km trajectory. There are significant differences, but if this were the whole picture, we should question whether the calculational pain of running the full CASCADE model is worth the results.



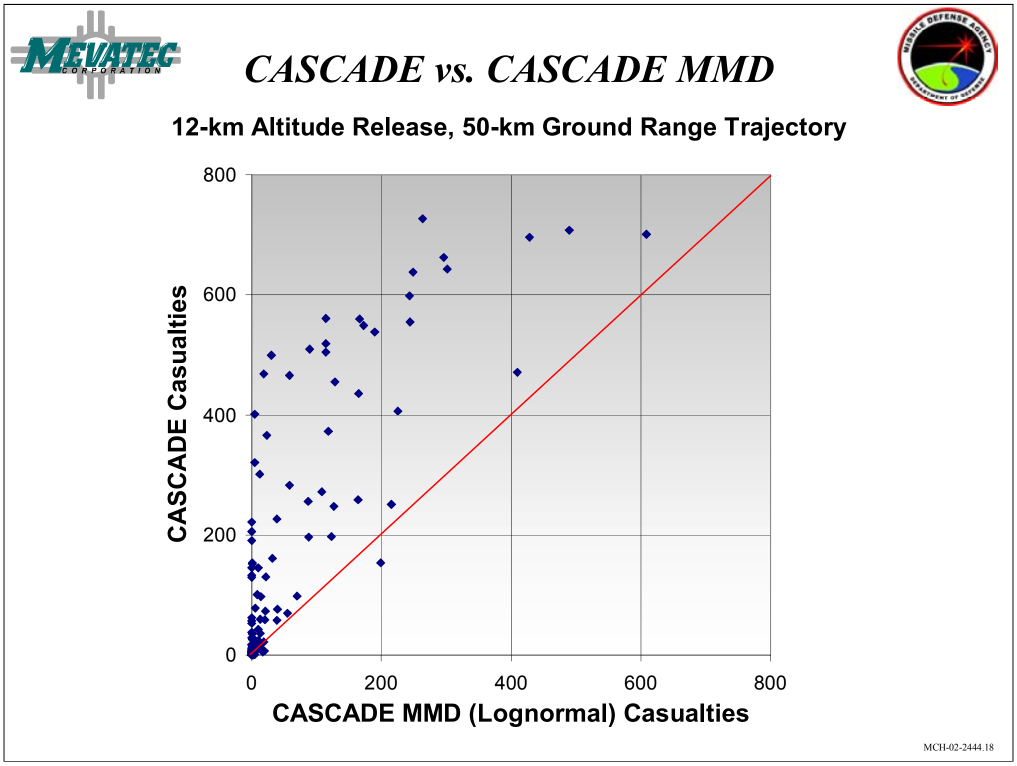
So let's look beyond that picture. Now the interest is at 12 km, still on the 500-km trajectory. Both models rarely yield a large number of casualties, but these is a very clear bias for the large drops in the CASCADE model to yield a greater number of casualties than Soltisz, even though the Soltisz MMD is greater than CASCADE's by over 50%.



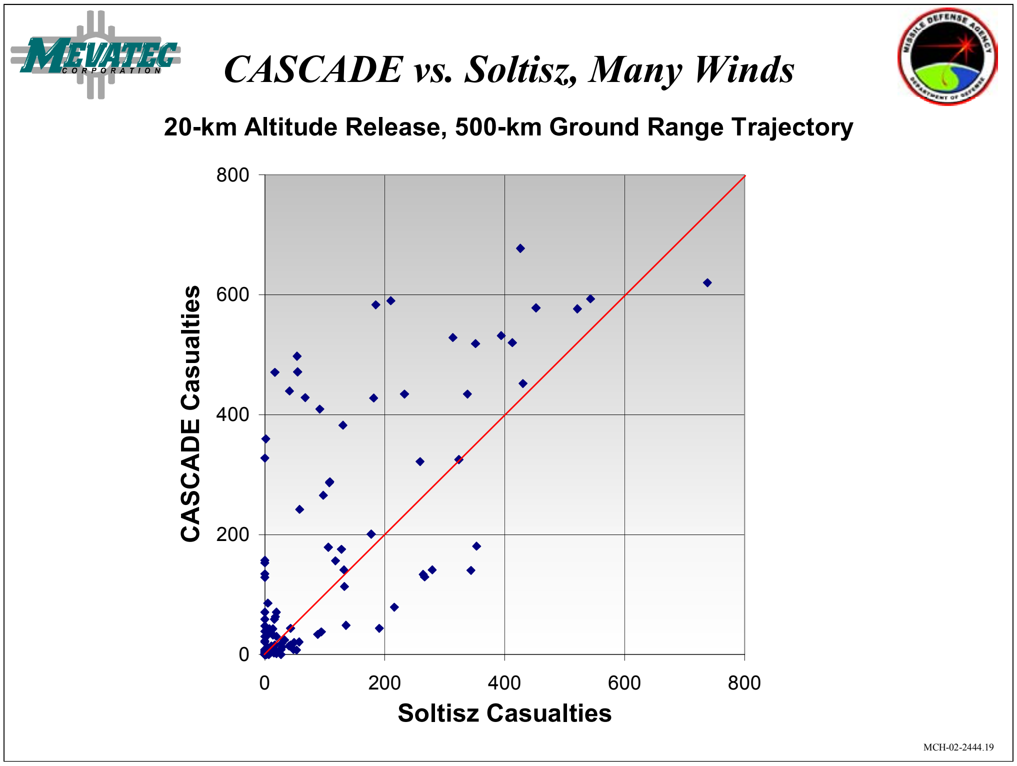
Still at 12 km altitude and 500-km range, now we also see that the large drops in the CASCADE distribution yield a reliable bias for greater casualties than when using the simpler lognormal distribution with the same CASCADE MMD. Now we have much stronger evidence that the calculational pain of the full CASCADE model might be worth the effort.



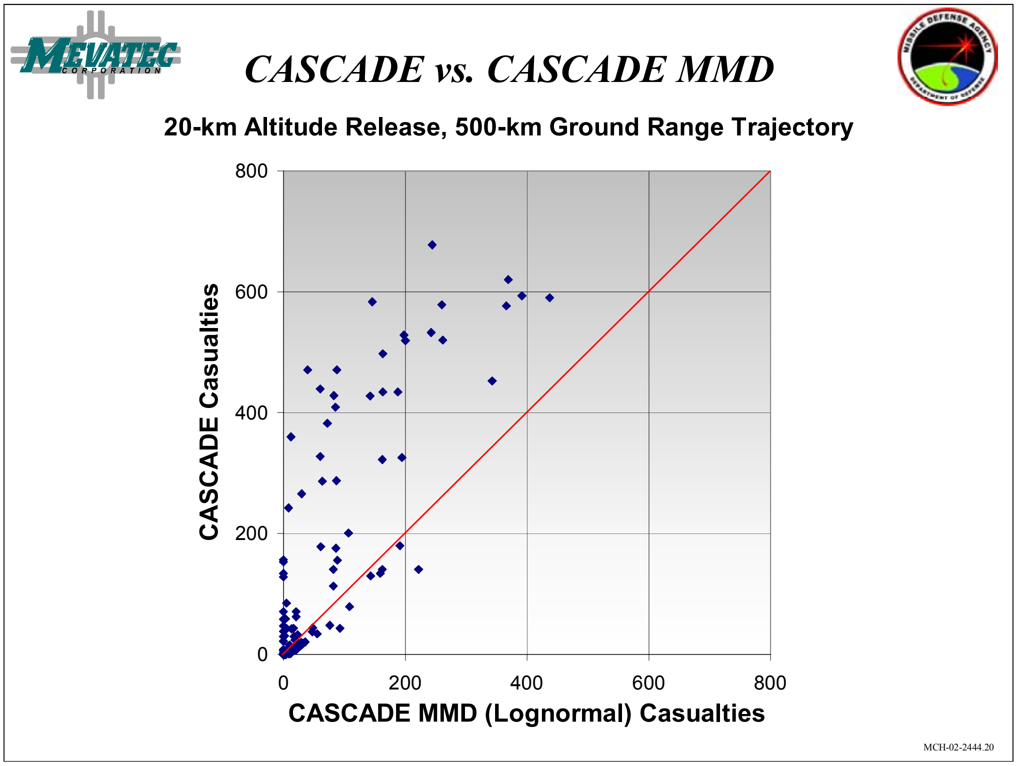
Switching now to the 50-km trajectory, still with a 12-km altitude, the Soltisz casualties are greater than the CASCADE because of the much greater MMD of the Soltisz model for this short-range trajectory. This plot is interesting principally because the CASCADE and Soltisz trends run so counter to one another: as the Soltisz casualties increase, the CASCADE casualties decrease. Unfortunately, I don't have a good explanation for this.



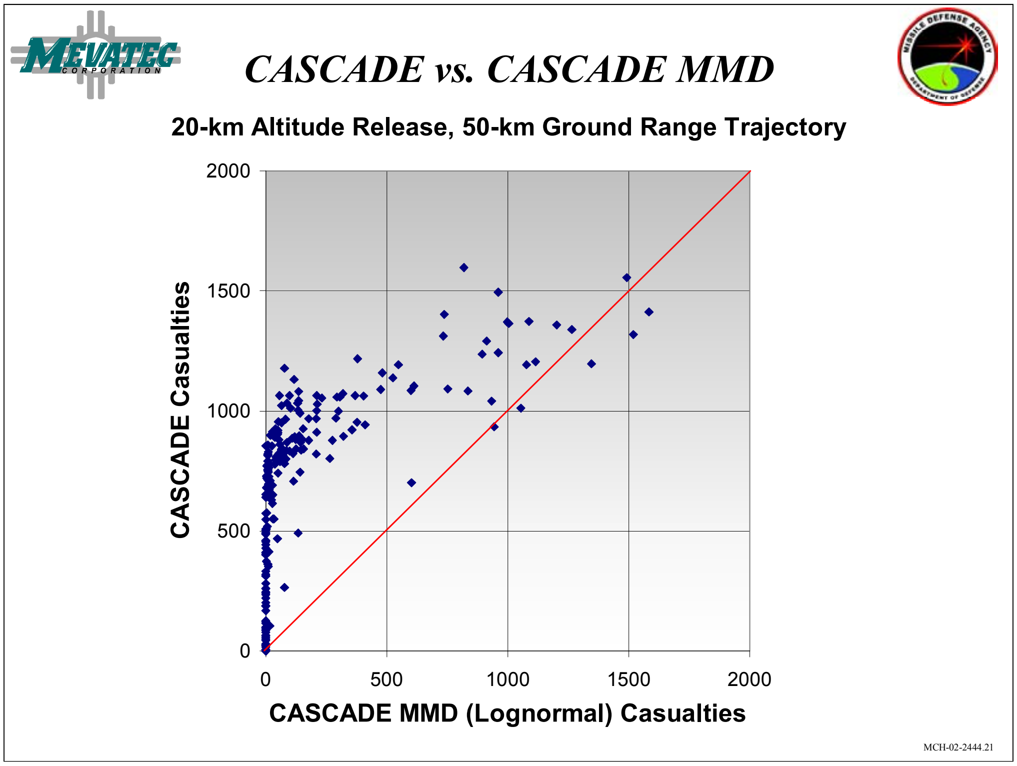
But this plot, still with the 12-km intercept and the short-range trajectory, is further evidence that the details of the distribution shape are important. The larger fraction of large drops in the raw CASCADE distribution yields greater casualties than a lognormal distribution with the same MMD and a matched sigma.



Finally I have three slides for intercepts at 20 km. The first two are for the 500-km trajectory. Here, the CASCADE versus Soltisz results are mixed, with a bias favoring the the large drops in CASCADE, though most results from both codes have few casualties. Note that an analysis with the Statistical Casualty Model in PEGEM would be expected to increase the bias towards higher CASCADE casualties.



The CASCADE versus CASCADE MMD results have the expected bias toward the larger fraction of large drops in the raw CASCADE distribution, though surprisingly there are a few exceptions.



Finally, with the short-range trajectory, we see again the strong bias toward the large drops in CASCADE, compared to the lognormal distribution with the CASCADE MMD.

Conclusions

- As already well established, ground hazards from bulk chemical releases are **sensitive** to the agent **drop size**.
- The **shape of the distribution** is also a significant factor.

  The large drops in CASCADE distributions can be important, increasing the hazard from intercept-induced releases. A lognormal with the same MMD may **underestimate** the severity of the hazard in these cases.
- Lack of an accurate drop distribution implies potentially large uncertainties in ground hazard predictions.

Caution: CASCADE results are sensitive to our assumed parent source terms and have not been validated.

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Here are our conclusions.

It is no surprise, but it is worth stating again that the ground effects resulting from a bulk chemical release are very sensitive to the agent drop size. However, a new twist to that observation is that we now see that the details of the shape of the droplet size distribution can be important, even if two distributions have the same MMD. The CASCADE distributions have a larger fraction of large droplets than do lognormal distributions build with the same MMD and a matching sigma, and this usually results in more severe ground effects. Finally, a logical conclusion from either one of the two preceding observations is that uncertainty in the droplet size distribution implies uncertainty in the expected ground effects. So if we are concerned with an accurate prediction of the ground hazards to result from a bulk chemical release, we must have confidence in our prediction for the droplet size distribution resulting from aerodynamic breakup.

Do you have any questions?