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**A Method for Sensitivity Analysis of Ground Protection
Afforded by Endoatmospheric Intercept of
Chemical Weapons**

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March 2001

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ABSTRACT

We have developed preliminary estimates of the protection afforded on the ground from releasing chemicals at altitude in the atmosphere and have used such estimates to determine the sensitivity of the protection to major variables such as wind speed, release altitude, drop size distribution, and turbulent dispersion. The approach used can be applied to provide detailed quantitative sensitivity analyses for each of the variables considered here. Preliminary sensitivity analysis indicates the most important variable affecting protection on the ground in all conditions and all altitudes of release is drop size distribution. We find that the drop size distribution so dominates the other variables that for a lognormal drop size distribution varying the truncation width assumed for the distribution produces larger variations in protection on the ground than the typical range of either release altitude or wind speed. The sensitivity analysis indicates the most important factor affecting ground deposition is drop size distribution. These results suggest that understanding and measuring the initial drop size distribution can reduce uncertainty concerning protection on the ground.

Work performed under the auspices of the U. S. Department of Energy by the Lawrence Livermore National Laboratory under contract W-7405-Eng-48.

1. Introduction

Lower tier TMD systems that successfully intercept targets carrying chemicals will likely release significant fractions of the chemical payloads into the atmosphere at or near the altitude of intercept, which for an edoatmospheric interceptor means somewhere between about 5 km and 35 km altitude. A major goal of missile defense is reducing the amount of the target's chemical payload that reaches the ground to levels that reduce the effects of the chemical to tolerable levels. Here we provide a quantitative and defense conservative estimate of the protection from ground deposition provided by release at altitude and provide a first order sensitivity analysis of chemical agent deposition on the ground to major determinants such as release altitude, drop size distribution, wind speed, and atmospheric turbulence. Details of the calculation and some other results can be found in [11].

2. Outline of the Problem

We restrict our attention to agent released as a cloud of spherical drops at some altitude and consider the dynamic effects of the drops falling to the ground. The canonical problem we consider is illustrated in Figure 1, which shows a cloud of chemical at altitude h over a point on the ground taken to be the origin of a cartesian coordinate system with altitude Z and ground distances Y and X . The chemical cloud has total mass M_0 and is distributed as spherical drops of various diameters D , with small initial relative velocity directed downward. We consider here only lognormal drop size and mass distributions, but the method easily applies to other distributions as well. We consider the collection of drops to be contained within a small volume relative to the altitude and displacements on the ground. To reach the ground, the drops fall by accelerating/decelerating under gravity to terminal velocity V_T and by maintaining V_T as a function of altitude, drop diameter, and speed relative to the ambient air. The drops remain at rest relative to the horizontal wind of magnitude V_w , which displaces the drops along the direction of the mean wind, here taken to be the X direction. The drops are displaced in the X and Y direction by atmospheric turbulence, which we assume results in a gaussian probability density of drop distribution in the X and Y direction. We calculate a quantity we call the deposition efficiency, denoted here by $R(D, X, Y, V_w, \sigma_w)$, which is the fraction of the chemical agent deposited per unit area on the ground at displacement (X, Y) from the origin.

$$\text{Deposition (mass/area)} = M_0 R(D, X, Y, V_w, \sigma_w)$$

It will sometimes be useful to use a measure we call protection, \mathbf{P} , afforded a point which we define as $-\log_{10}(R)$. For non-zero wind the displacement is a function of the drop size and R can be expressed as a function of either drop size or displacement.

We focus on the deposition efficiency, \mathbf{R} , as the measure of effectiveness for chemical release at altitude for several reasons. First, it is independent of agent type and exposure levels. Toxicity estimates for humans vary widely as a function of agent type, exposure pathway, and toxicity type [1,2]. Further, the human toxicity estimates necessarily result from limited data and consequently have relatively large uncertainties. Therefore a measure of effectiveness that incorporates toxicity would mask the defense effectiveness in the toxicity and agent variations.

Second, such factors are common measures of effectiveness for passive defense mechanisms such as filters, respirators, etc. and using it for missile defense allows ready comparison with other means of defense. Third, it is independent of the target total payload mass M_0 , which isolates the effects captured in R to effects of the defense alone, independent of the target characteristics. Fourth, when multiplied by M_0 , R immediately provides the dosage, in mass per square meter, that is relevant for percutaneous liquid exposure, of particular interest for this problem. A disadvantage of R as a measure of effectiveness is that it does not capture the time dependent dose rate effects important for other exposure routes and forms such as vapor inhalation.

A useful benchmark value for R is 10^{-8} , $P = 8$, which corresponds to the protection factor required to reduce to 1 mg/m^2 the deposition on the ground from the release of 100 kg of agent.

By using a simple model as described, we aim to provide a defense conservative estimate of defense effectiveness against chemical agents, independent of complicating effects, such as detailed meteorology and population distributions on the ground, which nevertheless captures key sensitivities. Not only is the weather notoriously variable as a function of location and time, but the effect of weather (wind and turbulence) tends to disperse the chemical cloud and work in favor of the defense. Our primary interest is determining the relative order of magnitude dependence of protection afforded as a function of major physical determinants.

3. Wind Dispersion

Consider releasing an agent cloud at any altitude in the range we are considering directly above the origin at (0,0), but in an ideal stable atmosphere (we use the U.S. Standard Atmosphere of 1976). If we imagine dropping each drop independently until all the mass is exhausted so that interference among drop descents is absent, it is clear that all of the mass will land on (0,0) and little protection is afforded that point. (It is reported that initial cloud extent may be a function of altitude, material type, and engagement details but generally is contained within a volume of major diameter of order tens of meters and no larger than a few hundred meters [3]. Since we will be concerned with displacements due to wind of many kilometers and we desire to be defense conservative, we neglect the spatial extent of the cloud at release.) Now if we generalize slightly by adding a **constant** wind, the drops are displaced down wind a distance depending on the wind speed and the fall time of the drop. If the drops are all exactly the same size, then all the drops again fall on the same point, this time just displaced down wind and little protection is afforded. If the drops are different sizes, then they have different terminal velocities and therefore different fall times. This causes faster drops to be displaced less distance down wind than slower drops, spreading out the drop impacts on the ground along the down wind axis. In this simple release, the protection would be a function of the fall time (release altitude and drop size), the wind speed, and the drop size distribution.

The relevant equation of motion for the spheres in the atmosphere is

$$\frac{Gm_D \vec{r}_D}{R} - \frac{1}{2} \rho_A C_D A \vec{V}_A V_A = m_D \dot{\vec{V}}_D$$

(1)

where m_D is the drop mass
 \mathbf{r}_D is the drop position vector
 R is distance from the earth center
 G is the gravitational constant
 ρ_A is the density of the air
 C_D is the drag coefficient for the drop
 A is the cross sectional area for the drop
 V_A is the velocity of the drop relative to the air ($V_D - V_w$)
 Dot denotes the time derivative.

The drops rapidly come to rest with respect to the wind and reach terminal velocity in the downward direction, defined by

$$V_T = \left[\frac{2m_D g}{\rho_A C_D A} \right]^{1/2} = \left[\frac{4\rho_D D}{3\rho_A C_D} g \right]^{1/2} \quad (2)$$

where g is the gravitational acceleration, $|Gr/R|$. For spherical drops, $A = \pi(D/2)^2$ and the mass of the drop is $m_D = \pi\rho_D D^3/6$ where ρ_D is the drop density so V_T can be expressed as a function of D , C_D , and the density ratio as shown. The drag coefficient for **rigid** spheres in air has been studied extensively [7] and is given in Figure 2 as a function of Reynolds number $Re = \rho_A D V_A / \mu$ where μ is the viscosity of the air. From equation (2) and C_D as given in Figure 2 we calculate (Figures 3 and 4) the terminal velocity as a function of altitude using the 1976 Standard Atmosphere for ρ_A and μ for two drop densities $\rho_D = 1008$ and $\rho_D = 2500 \text{ kg/m}^3$, representing chemical agent near the density of water and glass beads.

Under our assumptions that the drop falls at terminal velocity downward and at rest with respect to the horizontal wind, the displacement down wind for a drop falling from altitude h is just a function of the fall time and the wind speed as a function of time. We compute the displacement in two ways. We have integrated equation (1) numerically using MATLAB and use the numerical calculation for our analysis. One may also use a simple estimate of displacement as the product of the fall time t_{fall} and the wind speed V_w .

$$\Delta x \cong t_{fall} V_w \cong \frac{h}{V_t} V_w \quad (3)$$

In the estimate eq. (3) one can use the terminal velocity at 5 km altitude to represent an average value of V_T for the fall duration. Figure 5 shows the displacement as a function of drop size estimated by eq. (3) for release altitudes from 5 to 30 km and a wind speed of 5 m/s. Since only the product of h and V_w appears, the following altitude-velocity pairs have identical predicted displacements: (20km alt., 5 m/s speed), (5km, 20 m/s), (10km, 10m/s), etc. As can be seen from Figure 5, the simple estimate of eq. (3) agrees well with detailed numerical calculation. Consequently, one could obtain many of the results given below by using the simple approximation.

The chemical deposition (mass per unit area on the ground) is reduced because different size drops are displaced different distances during the fall according to equation (3). The reduction in the wind direction is expressed by

$$M(D)dD = M(D(x)) \left| \frac{dx}{dD} \right|^{-1} dx \quad (4)$$

Where $M(D)$ is the initial mass distribution with drop diameter D , x is the displacement on the ground and the derivative we calculate numerically or approximate as given via equation (3) by

$$\left| \frac{dx}{dD} \right|^{-1} = \left| h V_w \frac{1 dV_t}{V_t dD} \right|^{-1} = R_w \quad (5)$$

We define R_w as the protection factor due to the wind since it expresses the reduction of deposition due the mean wind effect on the chemical. For the estimates presented here, we calculate R_w numerically.

Mean zonal wind speed in the atmosphere is observed to vary with location, season, and altitude. In the altitude range from 5 to 35 km, reports of mean zonal wind speed as a function of altitude range in magnitude from 0 to as much as 100 m/s with sign changes as altitude increases being common [4]. Typical magnitudes are from 0 to 20 m/s. Our estimates here use a constant wind speed with altitude, which can be thought of as representing the average wind speed for the duration of the fall.

4. Turbulent Dispersion

We regard the wind as having a steady component (e.g. the mean wind described above) and a superimposed fluctuating component which produces stochastic gusts and lulls, that over time disperse a material in the atmosphere. The fluctuating component arises from turbulence phenomena that are much studied owing to their importance for understanding such phenomena as pollution sources and effluent from accidents [eg reference 5 for a review]. Characterizing and modeling turbulence at a detailed level can require a combination of extensive analysis, extraction of coefficients from experimental data, and intensive computational resources [6]. The results are typically characterized by a gaussian distribution of material in space, with standard deviations derived from fluid dynamic considerations. Here we are interested in quantifying the effect of turbulent dispersion on the effectiveness of release at altitude so we use a simple characterization of the effects of turbulence that grows with time roughly in accord with simple models and limited experimental data. In particular, we assume that the lateral dispersion of the cloud is given by

$$\sigma_{x,y}(D) = A \sqrt{\frac{t_{fall}}{t_v}} = \sigma \sqrt{t_{fall}} \quad (6)$$

Here $\sigma_{x,y}$ is the standard deviation of the material distribution in the x and y directions after fall time t_{fall} and we choose the constant σ_0 to be 10 meters per root second to match published data in order of magnitude [e.g. ref. 6]. Eq. (6) is motivated by the considering 1) that we are interested in relatively long time behaviour of the dispersion, and 2) that analytical (random walk) and empirical (2nd order closure) models approach $T^{1/2}$ form at long times, [5,6,10]. Ref [11] shows the result of gaussian dispersal according to eq (6). Note that the gaussian dispersal cannot be compared immediately with the wind dispersion because all the drop sizes in the gaussian case are dispersed randomly about the origin. The mass distribution with drop size must be incorporated into the estimate before comparisons can be made.

We incorporate the longitudinal dispersion of the material by convolving the wind dispersion amplitude at x with a gaussian defined as a function of x by the one to one correspondence of x with D. In particular we compute

$$R_w(x) = \int_{\min x}^{\max x} \tilde{R}_w(x') N(x - x', 0, \sigma(x')) dx'$$

Here $N(x, \mu, \sigma)$ denotes a normal (gaussian) distribution of a random variable x , with mean μ , and standard deviation σ . We have assumed for this analysis that the wind and turbulent dispersion mechanisms are independent.

5. Mass Drop Size Distribution

The lognormal distribution for a random variable x , $\Lambda(x; \mu, \sigma)$, where μ is the mean and σ the standard deviation of $\ln(x)$, has been widely applied to describe the particle size distributions from material breakup and formation of aerosols. The properties of the lognormal distribution are documented in [8] and discussion of the motivation and history of its application to breakup is found in [2 and 8]. It is current practice to use the lognormal distribution to describe the drop size distribution resulting from aerodynamic breakup in terms of the mass median diameter, $MMD = \exp(\mu)$, i.e. $\Lambda = \Lambda(D; MMD, \sigma)$. Experimental evidence is hard to obtain to establish the lognormal nature of the distribution of chemical agents following impact at altitude, and in practice [9], computer codes that generate drop distributions for dispersal codes typically use a value of $\sigma = 1.8$ and truncate the distribution between

$$D_{LowerBound} = MMD\sigma^{-4}$$

$$D_{Upperbound} = MMD\sigma^3$$

For these special assumptions, $M(D(x))$ from equation (4) is given by

$$M(D; x) = M_0 \left[\int_{MMD\sigma^{-4}}^{MMD\sigma^3} D^3 d\Lambda(D; MMD, 1.8) \right]^{-1} D^3 \Lambda(D, MMD, 1.8) \quad (7)$$

for x between $D_{LowerBound}$ and $D_{UpperBound}$ and zero elsewhere. Here M_0 is the total amount of mass in the target. We do not explicitly consider in-situ destruction in this analysis, apart from the physical effect of drop size distribution. The integral of Λ from lower to upper limits normalizes the expression to the truncated lognormal distribution.

We compute the deposition efficiency by numerically integrating the efficiency as function of drop size as computed using equation (4) over the mass drop size distribution as given in eq. (7) as

$$R_T(x, h, MMD) = \left[\int_{MMD\sigma^{-4}}^{MMD\sigma^3} D^3 d\Lambda(D; MMD, 1.8) \right]^{-1} \int_{MMD\sigma^{-4}}^{MMD\sigma^3} N(x, 0, \sigma(D)) N(y = 0, 0, \sigma(D)) D^3 d\Lambda(D, MMD, 1.8) \quad (8)$$

Where $N(x, \mu, \sigma)$ is the normal distribution at x with mean μ and standard deviation $\sigma(D)$ as given by eq. (6).

6. Sensitivity of Deposition to Key Variables

In this section we quantify sensitivity of deposition on the ground to the following variables and effects

- Drop diameter distribution
- Constant wind speed
- Release altitude
- Turbulent dispersion

Some of the effects we neglect are

- Drop evaporation
- Non-sphericity of drops
- Variations in weather
- Deactivation of chemicals at the point of release

Note that the effects neglected tend to reduce the deposition on the ground so that the estimates we present should be considered defense conservative, primarily useful for comparing the importance of one effect to another and to characterize trends due to the effects studied.

We work with the deposition efficiency afforded on the ground at various distances from the origin under various conditions and use units of per meter squared. Figure 6 shows a typical calculated case for release at 20 km altitude, MMD 1500 μ , wind speed 4 m/s and turbulent σ 20 $\text{m/s}^{1/2}$. The contours shown are contours of protection P. It is useful to relate deposition efficiency per meter squared to deposition by converting to milligrams per 100 kg payload per meter squared, i.e. multiplying by 10^8 . Severe and lethal human-toxicity estimates for VX agent are on the order of 1mg/70 kg person[1], which roughly corresponds to 1mg/m^2 , making a deposition efficiency of 10^{-8} ($P = 8$) a useful benchmark of utility.

We computed deposition efficiency for about 2600 cases spanning the ranges of release altitude, wind speed, drop size distribution MMD, and turbulent dispersion. The cases computed are shown in Figure 7. We compute three measures of effectiveness (MOEs), the minimum protection, the area with minimum protection less than 8.5 (the exposed area) and the displacement on the ground of the minimum protection from the origin (directly below the point of intercept), denoted maxX. The minimum protection (minP) measures the worst exposure of any point on the ground. The area with minP less than 8.5, denoted $A_{8.5}$, measures the amount of ground area exposed to depositions exceeding a threshold. These measures are illustrated in Figure 7 for the particular case shown.

We examine the sensitivity of the MOEs to key variables by statistical analysis of the 2600 cases computed. We evaluate both minP and maxX in terms of the key variables h , MMD, v_w , and σ by multivariable regression analysis. The variation of these measures is well explained by such models. Figure 8 shows a normal probability plot of the residuals of the regression of minP and indicates that most of the variation in the residuals is explained by the model and that the assumption of normal error distribution is reasonably well justified.

6.1 Sensitivity of MinP to Key Variables

We can examine the sensitivity of minP to the key variables by evaluating the differential change in minP due to nominal 10% increases in the variables. The result is shown in Figure 9. Increasing altitude, wind speed and turbulent dispersion by 10% all result in increasing minP by about 0.5, corresponding to a decrease in worst deposition by a factor of 1/3. Increasing the MMD by 10% results in a decrease in minP of about 0.7 or an increase in worst deposition by a factor of about 5. The signs of the differential changes accord with physical intuition that increasing altitude, wind speed, and turbulent dispersion should improve protection for the defense and that increasing the size of the drops should worsen protection for the defense.

Release altitude is of particular interest since the defense can choose, within bounds, whether to intercept higher or lower and thus affect the resulting dispersion of material. One common assumption has been that the higher the release, the better the protection afforded on the ground. Using the differential sensitivities in Figure 9, we can demonstrate that this assumption may not be warranted within the endoatmospheric range of altitudes. For given wind speed and turbulence, i.e. keeping v_w and σ constant, the changes in protection on the ground will be due to changes in h and MMD, which affect the protection in opposing directions. However, the physics of breakup indicates that release at higher altitudes will result in higher MMD which can potentially overcome the advantages of increasing altitude via atmospheric dispersion illustrated in Figure 9. We use published data and the differential sensitivity calculated here to estimate the importance of the tradeoff between dispersion and breakup

Breakup mechanisms result in higher MMD from breakup at high altitude. The left plot in Figure 10 shows several models of MMD resulting from aerodynamic breakup as a function of dynamic pressure. The models span values obtained experimentally [12] and provide a simple method for computing the tradeoff between breakup and dispersion. For a reentry velocity at release of 3 km/s, the dynamic pressure decreases with increasing altitude and according to the models in Figure 10, the MMD increases with altitude. The right plot of Figure 10 shows the result of combining the effects of breakup and dispersion on minP. Note that increasing minP reduces the magnitude of the worst exposed point on the ground and is therefore “good” for the defense. The plot shows that as altitude increases, the combined effects first improve protection in intermediate altitudes and then worsen protection at higher altitudes. This may mean that in some cases protection would be improved by intercepting at a lower altitude within the endoatmospheric range.

6.2 Sensitivity of Minimum Protection to Drop Size Distribution

Protection is remarkably sensitive to details of the drop size distribution assumed, in particular, the limits chosen for truncation. We arbitrarily changed the upper and lower limits used in eq. 7 in multiples of $\sigma = 1.8$, symmetrically for upper and lower limits and computed the resulting deposition efficiency. The results are shown in Figure 11. Changing the upper and lower limits about a given MMD can change the deposition efficiency by more than an order of magnitude for a case which is still characterized by the same MMD, wind speed, release altitude, and turbulence characteristics.

Sensitivity to drop size distribution is discussed in more detail in [11].

6.3 Sensitivity of Protected Area

The dependence of exposed area on altitude, wind speed, MMD, and turbulence is more complicated than that of minP and maxX and is currently under study. One can visualize the deposition as a function over area in which the height of the function is proportional to the protection. The shape of this contour is generally a wedge sharply pointed at one end, corresponding to the origin. The exposed area then is a slice along a particular value of the protection contour. The amount of area in the slice will depend on the difference between the threshold value and the value of minP for that case, on the turbulence in the atmosphere and on the dispersion. Figure 12 shows a scatter plot of the data that illustrates that exposed area generally decreases with increasing turbulence since the overall height of the contour is being reduced.

7. Conclusions

We have developed a method for estimating the deposition of chemical agents released at altitudes in the range from 5 to 35 km. We have used such estimates to determine the sensitivity of the protection to major variables such as wind speed, release altitude, drop size distribution, and turbulent dispersion. The approach used can be applied to provide detailed quantitative sensitivity analyses for each of the variables considered here. Preliminary sensitivity analysis indicates the most important variable affecting protection on the ground in all conditions and all altitudes of release is drop size distribution. We find that the drop size distribution so dominates the other variables that for a lognormal drop size distribution varying the truncation width assumed for the distribution produces larger variations in protection on the ground than the typical range of either release altitude or wind speed. While increasing MMD improves protection afforded on the ground via atmospheric dispersion, increasing altitude also apparently increases the MMD as a result of breakup physics and the effect of reducing dynamic pressure. A quantitative examination of the tradeoff between dispersion and breakup indicates that there may be intermediate optimal altitudes at which to intercept to minimize effects on the ground. These results suggest that understanding and measuring the initial drop size distribution can reduce uncertainty concerning protection on the ground.

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Figure 1

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Outline of the problem

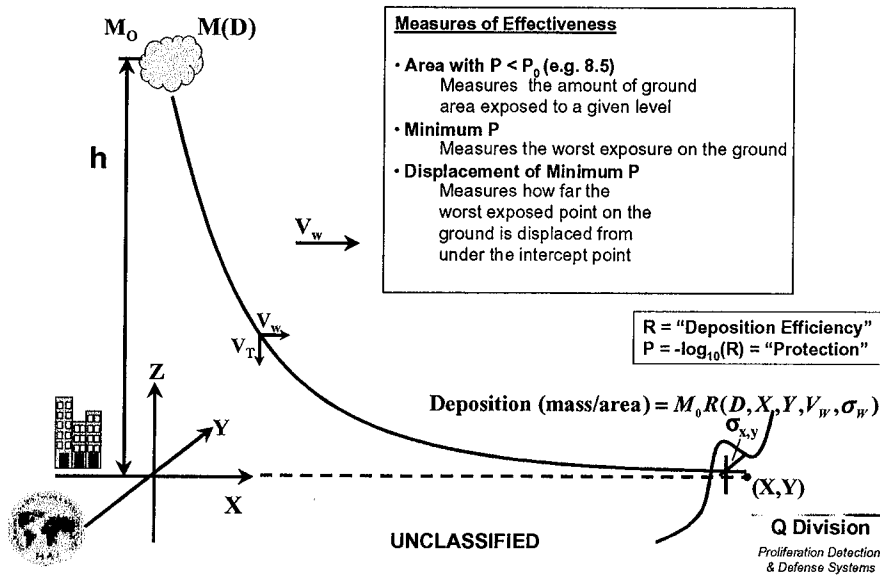
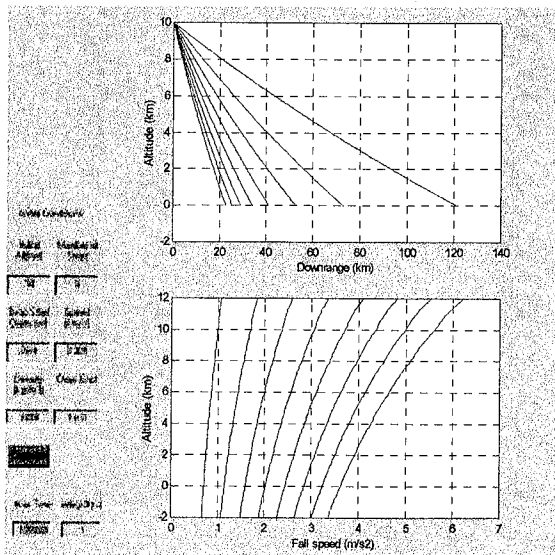


Figure 2.

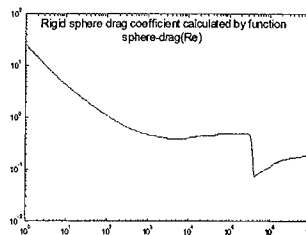
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Motivation: Understand Dispersion



Equations of Motion:

$$\frac{Gm_d \vec{V}_d}{R} - \frac{1}{2} \rho_a C_D A \vec{V}_d V_a = m_d \vec{V}_d$$



$$Re = \frac{\rho_a D V_a}{\mu}$$



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Figure 3.

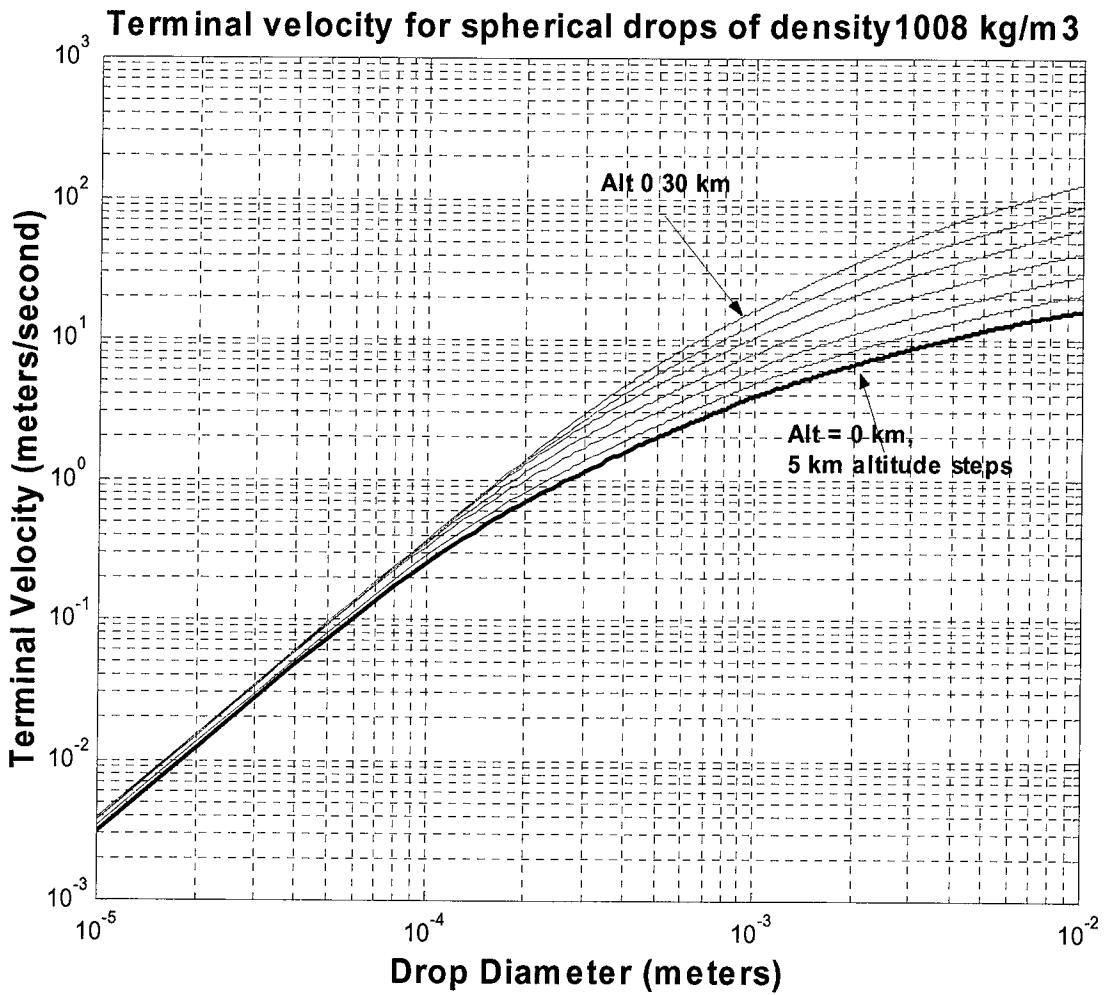


Figure 4.

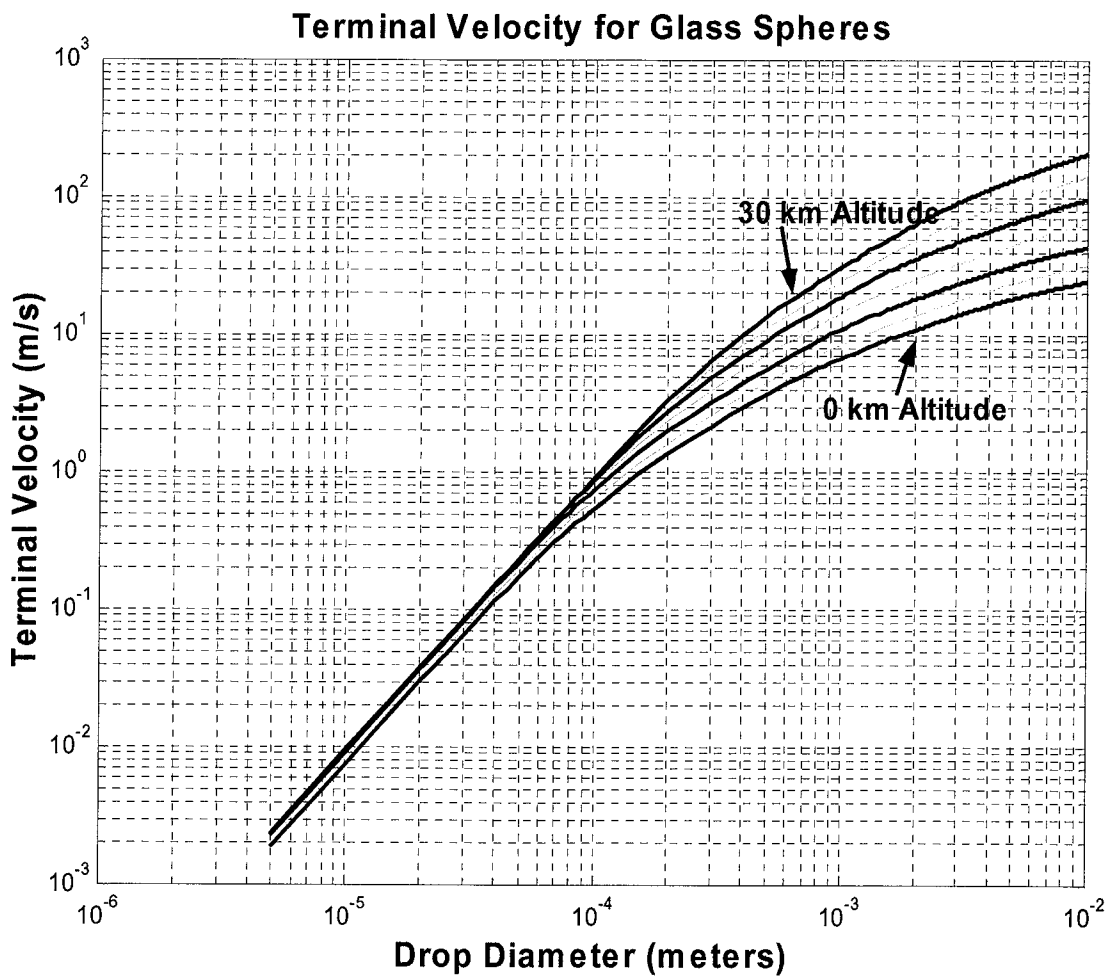


Figure 5

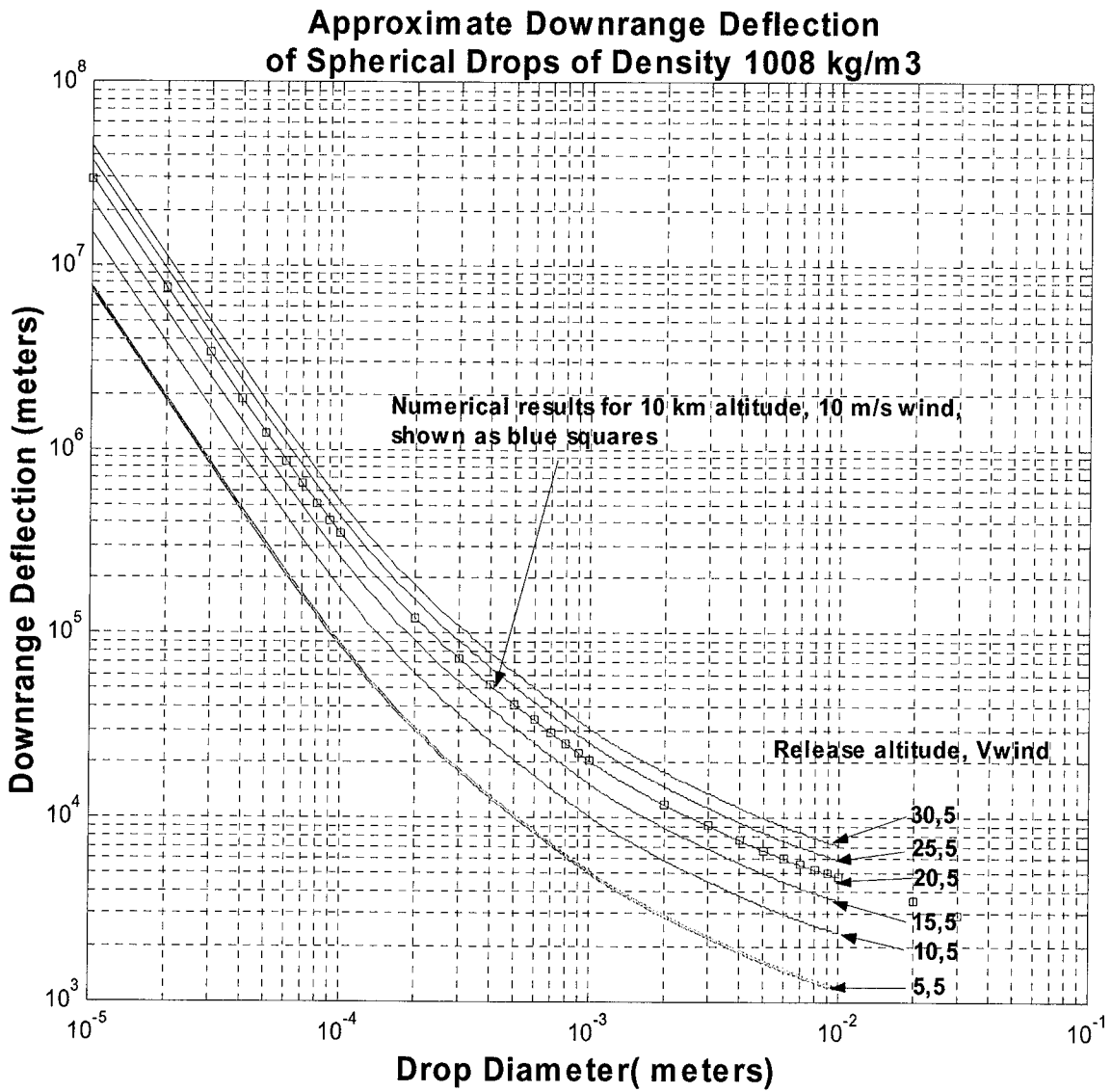
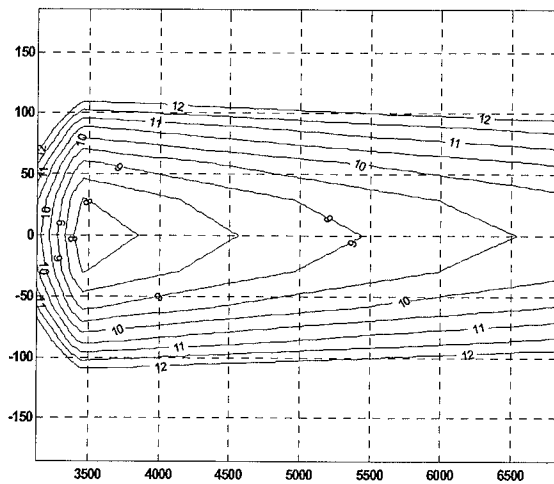


Figure 6

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Computed protection contour plot represents effectiveness of release at given conditions



- Measures of Effectiveness**
- Area with $P < P_0$ (e.g. 8.5)
5.3 x 10⁴ sq. m.
 - Minimum P
7.5
 - Displacement of Minimum P
3500 m

Contours show levels of protection = $-\log_{10}(R)$
= $-\log_{10}$ (fraction of released mass deposited per unit area on the ground)



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Figure 7

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2,600 cases span range of key physical variables

<u>Release MOEs Computed</u>	<u>Cases Computed</u>
<ul style="list-style-type: none">• Area with P < 8.5 Measures amount of ground area exposed to given level (Data stored allows other levels to be chosen)• Minimum P Measures the worst exposure on the ground• Minimum P Displacement Measures how far the worst exposed point on the ground is displaced from under the intercept point	<ul style="list-style-type: none">• Release altitudes:<ul style="list-style-type: none">– 5,10,15,20,25,30 km• Wind Speeds<ul style="list-style-type: none">– 1,2,4,8,16,32 m/s• MMD values<ul style="list-style-type: none">– 100,120,140,160,180, 200,400,600,800,1000, 1200, 1500 μ• Turbulent dispersion σ_0<ul style="list-style-type: none">– 2,5,10,20,40,60 m/s^{1/2}



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Figure 8

Residuals of Regression of Min P on h, v, MMD, and σ

Normal Probability Plot

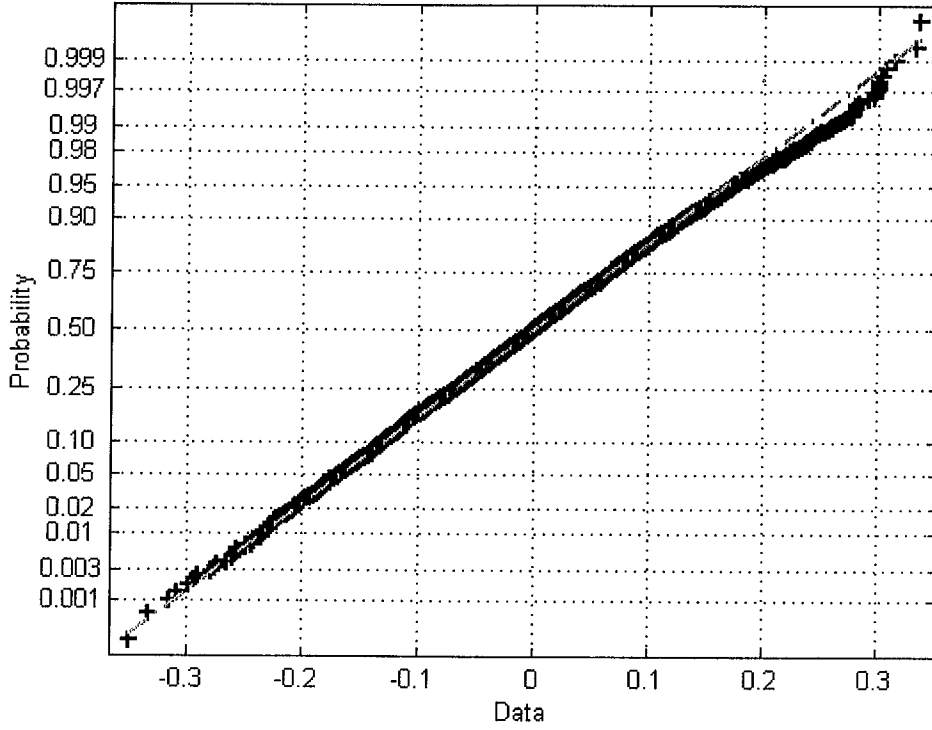
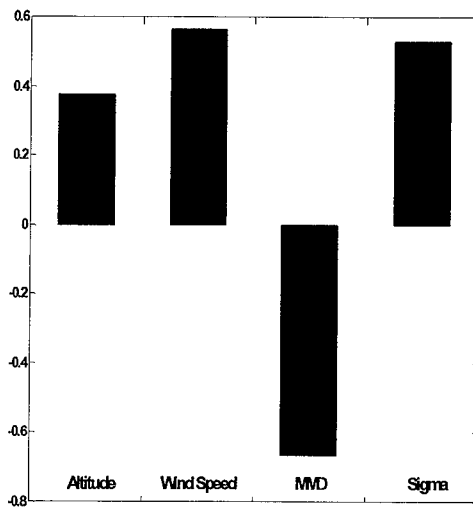


Figure 9

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Differential sensitivity of Minimum P follows physical intuition



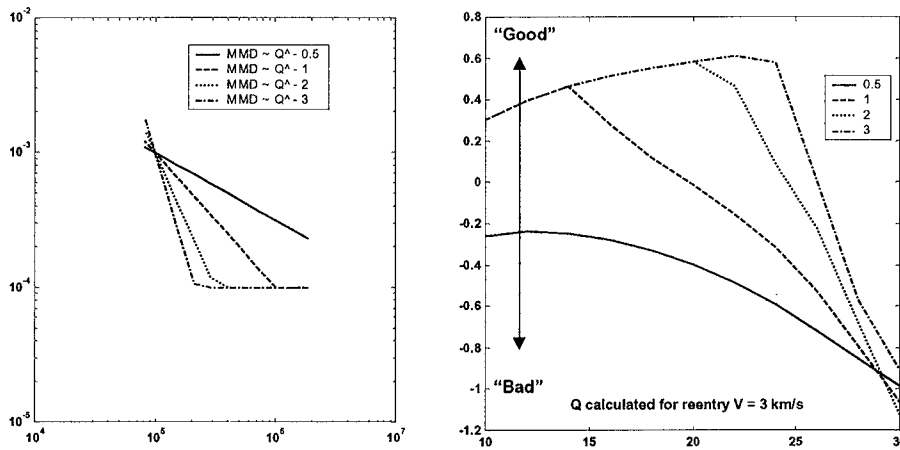
2600 Cases Computed

- Release altitudes:
 - 5,10,15,20,25,30 km
- Wind Speeds
 - 1,2,4,8,16,32 m/s
- MMD values
 - 100,120,140,160,180, 200,400,600,800,1000, 1200, 1500 μ
- Turbulent dispersion σ_0
 - 2,5,10,20,40,60 m/s^{1/2}



Figure 10

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Benefit of increasing release altitude depends on details of material breakup physics



Trend of altitude is to provide worse protection as altitude increases but breakup physics can delay protection degradation to higher altitude.

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Figure 11

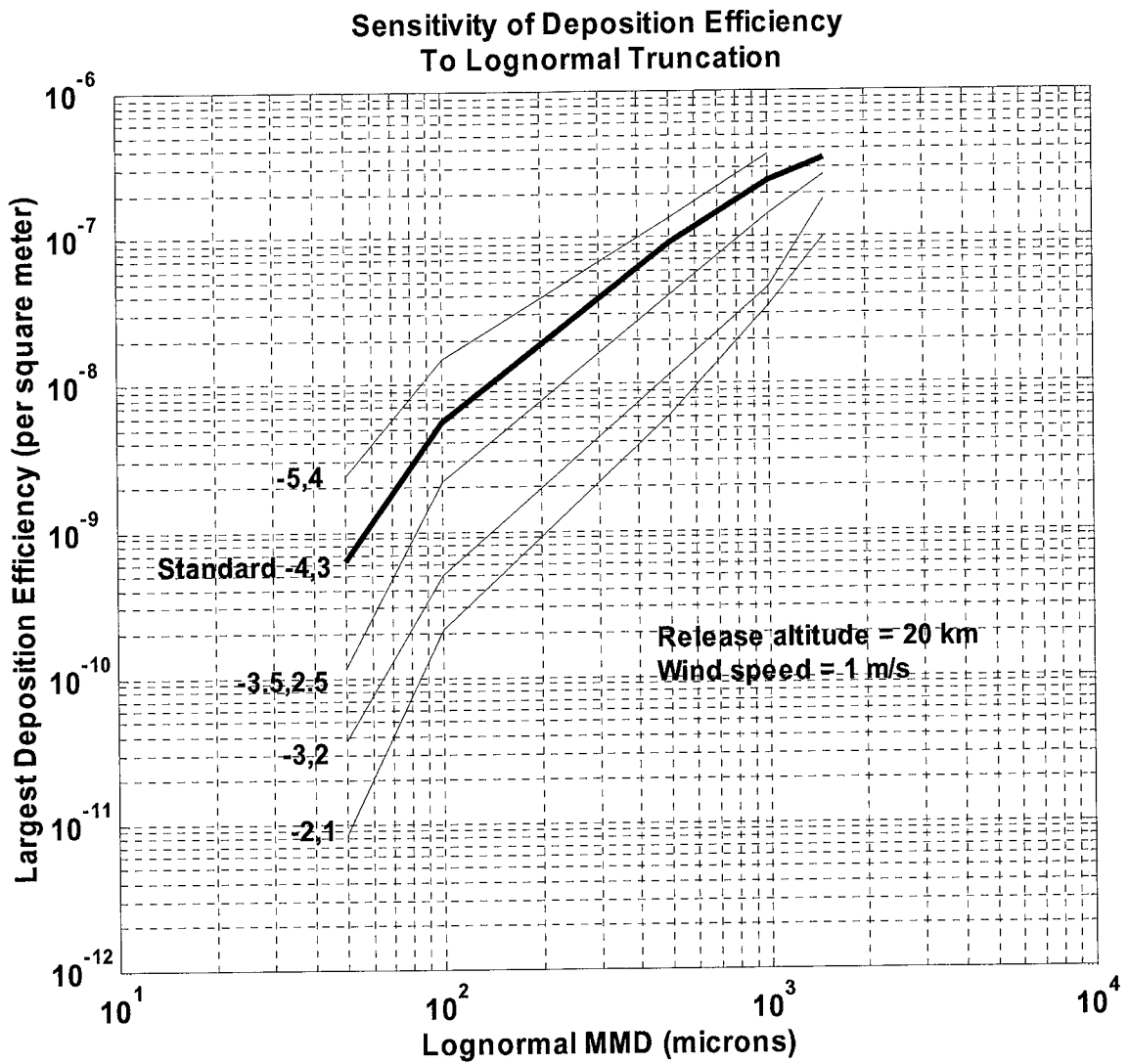


Figure 12

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Area exposed has clear dependence on key variables but a model requires further study

