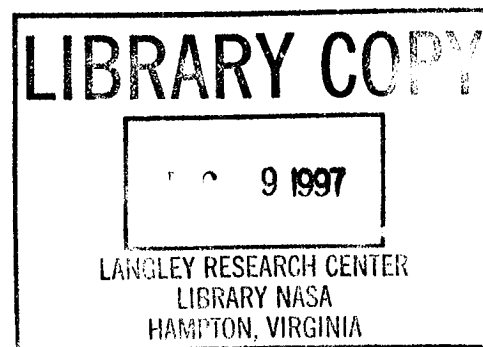


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REVIEW AND DEVELOPMENTS OF  
DISSEMINATION MODELS FOR  
AIRBORNE CARBON FIBERS

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## SUMMARY

Dissemination prediction models have been reviewed to determine their applicability to a risk assessment for airborne carbon fibers. The review showed that the Gaussian prediction models using partial reflection at the ground agreed very closely with a more elaborate diffusion analysis developed for this study. For distances beyond 10000 m the Gaussian models predicted a slower fall-off in exposure levels than the diffusion models. This resulting level of conservatism was preferred for the carbon fiber risk assessment. The results also showed that the perfect vertical-mixing models developed herein agreed very closely with the diffusion analysis for all except the most stable atmospheric conditions.

## INTRODUCTION

This study of dissemination models was made to support a risk assessment of carbon fibers released in aircraft accidents.

Carbon fibers have light weight, high strength, and high stiffness and are being used together with epoxy resins to form composite materials. These materials may appear in large amounts in aircraft structures of the future. But the fibers have disadvantages, too. Their electrical conductivity has caused electrical equipment failures in the manufacturing process, and similar problems are likely to occur if the fibers are released from the composite. That could occur if the material is burnt in an aircraft accident. The risk study for that problem (ref. 1) involved the analysis of the atmospheric transport of the fibrous particles. The study reported here is a part of that effort; it represents a review of the existing dissemination models, their applicability, and some developments of simple models suitable for closed form mathematical analysis of such problems.

The dissemination of lightweight particles and gases in the atmosphere has been studied both analytically and experimentally and involves disciplines such as fluid mechanics, meteorology, and statistics. An early summary text of the subject was prepared by Pasquill (ref. 2). The main phenomena which must be accounted for in a dissemination analysis are turbulent mixing in the convection layer of the atmosphere, the downwind transport with the wind, and the falling of heavier-than-air particles. All of these processes are stochastic; therefore, the variables which must be predicted--such as concentration at a point--have statistical distributions with wide variability. Only the long term averages can really be quantified by any simple mathematical model. Figure 1 shows a smoke plume from a fire test in which structural components made with carbon fibers were burnt so that the fibers could be released. Such a smoke plume can be idealized near its source as a conically expanding point source as shown by the solid lines.

The simplest mathematical models that describe the particle dissemination are the Gaussian models such as the Turner model (ref. 3), and the Cramer models (ref. 4). They are based on the fact that a point source of particles will produce such a conically growing particle cloud with a Gaussian transverse concentration profile. The growth is limited by the thin turbulent air layer between the ground and the inversion layer. The Gaussian models simply use a light beam reflection analogy to determine the growth of the Gaussian cloud beyond the point where the conically growing cloud first intersects either the ground or inversion planes. The falling of heavier-than-air particles and their deposition on the ground are simulated by making the ground reflectivity imperfect and by tilting the initial conical cloud at an appropriate fall angle.

The more complex models are the particle-in-a-cell models (refs. 5 and 6), which solve the turbulent mixing, the downwind transport, and the falling in a three-dimensional analysis. The solutions can only be obtained numerically and require a large computer.

The assessment of the effects of carbon fiber dissemination from aircraft fires was made by thousands of repetitive simulation of potential accident scenes for a number of cities around the nation. In these simulations the weather was randomly assumed to be characterized by one of the six Pasquill-Gifford stability classes (ref. 1). The simple Gaussian models were computationally ideal for this repetitive application. They have been developed to predict exposures close to the source of pollution and such predictions had been experimentally verified for distances up to 10 km. But in the carbon fiber study these models were to be applied up to distances of 100 km. One purpose of this study was to assure that the models were accurate, and that the empirical constants describing the particle deposition were correctly modeled for carbon fibers.

This study recognized that there was little experimental data for diffusion at long distances and that because of the large variability of the atmospheric processes no single test series could be conducted to prove the accuracy of these models. Therefore, this study aimed to show analytically that these models are logically consistent and to determine if they satisfy the principle of mass conservations and an appropriate particle deposition law.

For that step, a diffusion model was set up which handles the assumed deposition law and the diffusivity limitations at the ground in an exact manner. The predictions of the two Gaussian models was then compared with the diffusion model at points within a small distance from the source. Also, the predictions from all models had indicated that the particle distribution in the vertical direction become uniform between the ground and the inversion. Therefore, an analytical model was set up in which a uniform vertical particle distribution was assumed. This model was used to show the parametric relation between the variables in the dissemination process and is useful for fast and simple exposure calculations. The derivation of all of the models are presented here and comparisons are made among the predicted results from the models.

## LIST OF SYMBOLS

|                                   |  |
|-----------------------------------|--|
| A                                 | area, $m^2$  |
| B                                 | integration constant   |
| C                                 | concentration, $f/m^3$                                       |
| C'                                | concentration parameter                                      |
| C <sub>o</sub>                    | initial condition for concentration, $f/m^3$                 |
| C <sub>x,y</sub>                  | concentration in Cartesian coordinates, $f/m^3$              |
| C <sub>+1</sub> , C <sub>+2</sub> | concentration in finite cells, $f/m^3$                       |
| C( $\epsilon$ )                   | concentration at height $\epsilon$ , $f/m^3$                 |
| D                                 | deposition density, $f/m^2$                                  |
| E                                 | exposure, $f\text{-}s/m^3$                                   |
| e                                 | experimental constant, 2.71828                               |
| F <sub>1</sub> (y,t)              | crosswind dispersion function                                |
| F <sub>2</sub> (z,t)              | vertical dispersion function                                 |
| F <sub>x</sub>                    | particle flux through a section of $x$ , $f/m^2 \cdot s$     |
| F <sub>y</sub>                    | vertical particle flux, $f/m^2 \cdot s$                      |
| G                                 | nondimensional function, $\beta/2\theta_E$                   |
| H                                 | height of atmospheric inversion, m                           |
| h                                 | source release height, m                                     |
| h <sub>o</sub>                    | initial condition for cloud height, m                        |
| I                                 | crosswind integral of concentration, $f/m^2$                 |
| I <sub>x,z</sub>                  | crosswind integral of concentration of coordinates, $f/m^2$  |
| I <sub>x,o</sub>                  | crosswind integral of concentration at ground level, $f/m^2$ |
| i                                 | integer coefficient  |
| j                                 | integer coefficient  |
| K                                 | diffusivity of the atmosphere                                |

$K_y$  crosswind diffusivity  
 $K_z$  vertical diffusivity  
 $K_{\epsilon/2}$  diffusivity between adjacent cells  
 $k$  integer coefficient  
 $N$  total number of particles  
 $n$  summation counter  
 $\dot{n}$  particle release rate  
 $\dot{n}_x$  particle flux through a section  $x$   
 $\dot{n}_0$  initial condition for particle flux, f/s  
 $p$  constant in diffusivity equation  
 $q$  air flow  
 $q_{0,1}$  air flow between two adjacent cells  
 $q(\epsilon/2)$  air flow of height  $\epsilon/2$   
 $r$  reflection coefficient  
 $t$  time, s  
 $u$  mean wind speed, m/s  
 $v_a$  equivalent exchange flow velocity, m/s  
 $v_s$  particle free fall velocity  
 $x$  downwind coordinate, m  
 $x_{I_{max}}$  coordinate of maximum crosswind integral, m  
 $x_{C_{max}}$  coordinate of maximum concentration, m  
 $x_0$  coordinate for initial conditions, m  
 $y$  crosswind coordinate, m  
 $Z$  vertical coordinate relative to ground, m  
 $z$  vertical coordinate relative to cloud center, m  
 horizontal spreading angle

|            |   |
|------------|---|
| $\beta$    | relative fall angle                         |
| $\Delta$   | finite increment for any function           |
| $\epsilon$ | thickness of an air cell, m                 |
| $\gamma$   | vertical spread angle for rectangular cloud |
| $\phi(x)$  | cloud expansion function                    |
| $\theta$   | declination of a point $x$ below the source |
| $\theta_A$ | azimuth spread angle                        |
| $\theta_E$ | elevation spread angle                      |
| $\tau$     | nondimensional function                     |
| $\tau_0$   | initial condition for $\tau$                |
| $\sigma_y$ | dispersion in the crosswind direction       |
| $\sigma_z$ | dispersion in the vertical direction        |
| $\omega$   | width of a idealized cloud                  |
| $\omega_0$ | initial condition for $\omega$              |

## ANALYSIS

### Definition of Terms

Because this study deals with particulate pollution, the quantities of pollutants are treated by enumeration, rather than by volume or mass. The particle concentrations are given in terms of particles per cubic meter and are given the symbol  $C$ .

Many of the effects of atmospheric pollution are not just a function of the particulate concentration, but of the time-integral of concentration or the product of concentration and time. This quantity is termed either the exposure or dosage, has the symbol 'E,' and is measured in particle seconds per cubic meter.

Heavier-than-air particles may be tossed around by the turbulent atmosphere, but inside the turbulent cells of air the one constant force always acting on these particles is gravity, and it will move these relative to that air toward the ground at a mean fall velocity versus equal to that observed in still air.

Ultimately, all particles will deposit on the ground. The measure of ground contamination is the particle deposition density  $D$  measured in particles per square meter. The fact that all particles once airborne and contributing to the exposure must ultimately end up as a deposit leads to a mass conservation rule which all dissemination models should satisfy.

#### The Mass Conservation Rule

If particles fall with a mean fall velocity  $v_s$ , then they will deposit from a volume where the concentration is  $C$  at a rate  $Cv_s$  and, when all the particles have been deposited, the total deposition density will be

$$D = \int C v_s dt$$

or

$$D = E v_s$$

If a total of  $N$  particles were initially airborne, the sum of all the deposited particles over all areas where particles had spread must be

$$\int D dA = N$$

This is the mass conservation rule applicable to particle dissemination. If we combine this with the relation between exposure and deposition we get

$$\int E dA = N/v_s$$

That relation prescribes a limit to the total area coverage which can result from a source of  $N$  particles having free fall velocity  $v_s$ .

This rule should be satisfied by any dissemination model for heavier-than-air particles.

#### The Gaussian Models

For a continuous point source emitting particles at a rate  $\dot{n}$ , the diffusion in the vertical and crosswind direction leads to a concentration profile with Gaussian distributions in these two directions. If  $z$  is the vertical distance and  $y$  the crosswind distance from the centerline, then the concentration is



$$C = \frac{\dot{n}}{u \sqrt{2\pi} \sigma_z \sigma_y} e^{-y^2/2\sigma_y^2} e^{-z^2/2\sigma_z^2}$$

Because the functions are fully separable in  $y$  and  $z$  the concentration profile can always be obtained from the transverse or crosswind concentration integral (see appendix A) where

$$I = \int_{-\infty}^{\infty} C \, dy = \frac{\dot{n}}{u \sqrt{2\pi} \sigma_z} e^{-z^2/2\sigma_z^2}$$

and

$$C = I \times \frac{1}{\sqrt{2\pi} \sigma_y} e^{-y^2/2\sigma_y^2}$$

The reason for working with the crosswind concentration integral is that in most dissemination problems the dispersion in the crosswind direction is essentially unrestricted and the crosswind distribution can be assumed to remain Gaussian. In the vertical direction, the growth of the Gaussian plume becomes constrained by the lack of turbulent mixing into the inversion and the ground boundary layer. These complications are more easily solved by dealing with the crosswind integral  $I$ , which is independent of  $y$ .

The accommodation of the zero turbulence both at the ground and at the inversion in the Gaussian models is approximate. Inplace of solving the diffusion equations, they assume that the particle behavior near the ground is analogous to the behavior of a light beam reflected off the ground. Figure 2 shows a fiber source at a height  $h$  above the ground when the inversion is at a height  $H$ . The centerline of the "beam" is declined at an angle  $\beta$ . If the reflectivity at the ground is designated as 'r,' then at any point  $x$  downwind from the source and a distance  $Z$  above the ground, the contribution to the crosswind integral from the prime source is

$$I_{x,z} = \frac{\dot{n}}{u \sqrt{2\pi} \sigma_z} e^{-z^2/2\sigma_z^2}$$

where

$$z = h - \beta x - Z.$$

Those Gaussian models which use imperfect reflection to model deposition (ref. 7) are referred to as the Gaussian partial reflection models. The reflections of the prime source and the reflections of reflections contribute to the vertical distribution of crosswind integrals. It can be shown that if

$$i = \text{integer value of } n/2 = \text{INT } (n/2)$$

$$j = \text{INT } ((n - 1)/2)$$

$$k = \text{INT } ((n + 1)/2)$$

$$I_{x,z} = \frac{\dot{n}}{u\sqrt{2\pi} \sigma_z} \left\{ \sum_{n=1}^{\infty} r^i e^{-z_1^2/2\sigma_z^2} + r^i e^{-z_2^2/2\sigma_z^2} \right\}$$

where

$$z_1 = 2jH + h - \beta x + (-1)^n Z$$

and

$$z_2 = 2kH - h + \beta x + (-1)^n Z$$

The above equations represent the Gaussian partial reflection model, in which the partial reflection coefficient  $r$  must be empirically determined to fit the particle deposition rate. The process is best understood by an illustration of a slowly growing light beam.

Figure 3 is an isometric representation of the strength of the crosswind integrals at 10 downwind sections. The source beam has a Gaussian distribution defined by

$$\sigma_z = \theta_E x$$

It is a linearly growing 'beam.' The reflection coefficient is unity both at the ground and at the inversion. The light beam alternately bounces off the ground and off the inversion. As it spreads the distortion from the reflections slowly changes the distribution from a Gaussian to a uniform distribution. The total section flux at all sections is

$$F_x = u \int_0^H I dz = \dot{n}$$

as required for conservation of mass. In the particle dissemination problem the same physical reflection concept is applied to model the lack of turbulent mixing in the inversion and near the ground. The deposition of particles is modeled by partial reflection on the ground; and the fall velocity of the particles is modeled by inclining the cloud of an angle  $\beta$ , determined from the fall velocity and the wind velocity.

For the small spreading angle shown in figure 3, this modeling would not very satisfactorily describe the behavior of particles because the reflection actually changes the direction of fall leading to a net vertical rise velocity for the particles remaining airborne after the reflection. This represents an anomaly in the modeling which shows up most strongly for particles with high fall velocities in very stable weather conditions.

Unlike the example shown in figure 3, most particle dissemination problems have dispersion angles  $\theta_E$  larger than the fall angle  $\beta$ . For those problems the vertical distribution soon becomes uniform and the bouncing light beam effect of figure 3 is not visible in the solution. Figure 4 shows a solution for a dissemination problem in stable weather with the following parameters:

$$H = 100 \text{ m}$$

$$h = 50 \text{ m}$$

$$u = 1.5 \text{ m/s}$$

$$v_s = 0.02 \text{ m/s}$$

$$\theta_E = 0.025$$

$$r = 0.3$$

At the last section shown,  $x = 2000 \text{ m}$ , the distribution is almost uniform. The mean fall distance of the particles is 26.7 m as indicated by the solid centerline of the expanding plume. For the neutral and unstable weather categories the dispersion angle  $\theta_E$  is even larger and the distributions become uniform very much faster.

The location of the maximum exposures was important to the risk measurement and was obtained as an analytical expression here. It can be shown that the original source and its ground reflection contribute significantly to the maximum exposures at ground level. If the crosswind integral  $I_{x,0}$  consists only of these two terms, then

$$I_{x,o} = (1 + r) \frac{\dot{n}}{\sqrt{2\pi} \theta_E x} e^{-z^2/2\theta_E^2 x^2}$$

in which

$$z = h - \beta x$$

For this expression it can be shown that the maximum occurs at

$$x = \frac{h}{\theta_E} \left\{ \sqrt{1 + \frac{\beta^2}{4\theta_E^2}} - \frac{\beta}{2\theta_E} \right\}$$

or if

$$G = \frac{\beta}{2\theta_E} = \frac{v_s}{2u\theta_E}$$

$$x_{\text{Imax}} = \frac{h}{\beta} \times 2G \left\{ \sqrt{1 + G^2} - G \right\}$$

and if the lateral dispersion of the cloud is linear the maximum concentration of exposure occurs at

$$x_{\text{Cmax}} = \frac{h}{\beta} \times G \left\{ \sqrt{2 + G^2} - G \right\}$$

The use of the partial reflection concept for simulating particle deposition leads an anomaly. Conceptually we require that the deposition rate at the surface should be the product of concentration and fall velocity so that the crosswind integral of deposition rate should be  $I_{x,o} v_s$ . The total deposition between the source and section  $x$  is

$$\int_0^x I_{x,o} v_s dx$$

and the residual flux is

$$u \int_0^H I_{x,Z} dz$$

Mass conservation requires that the sum of these two integrals be equal to the particle flux  $\dot{n}$

$$\dot{n} = u \int_0^H I_{x,Z} dz + v_s \int_0^x I_{x,0} dx$$

The Gaussian models have a different relation governing deposition. This can be seen at small distances  $x$  where only the original source and its first reflection contribute to the ground level concentration.

Let

$$I_{x,0} = (1 + r) \frac{\dot{n}}{u\sqrt{2\pi} \sigma_z} e^{-z^2/2\sigma_z^2}$$

where

$$z = h - \beta x$$

The flux through the surface is a vector with a direction shown in figure 5, where

$$\theta = \tan^{-1}(h/x)$$

The net vertical component from the flux of the prime source and its first reflection is

$$F_y = (1 - r) \frac{h}{x} u I_{x,0}$$

Because this deposition flux has a different functional form ( $x$  in the denominator) than the desired deposition rate  $v_s I_{x,0}$  the Gaussian partial reflection model cannot satisfy the desired deposition rule, and the mass conservation rule simultaneously.

One alternative which had been used (ref. 8) is a Gaussian depletion model. That model uses full reflection of the particles, together with an overall depletion function such that

$$\dot{n}_x = \dot{n} - v_s \int_0^x I_{x,0} dx$$

and

$$I_{x,0} = \frac{n_x}{u\sqrt{2\pi} \sigma_y} e^{-z^2/2\sigma_y^2}$$

plus reflection terms.

The Gaussian depletion model satisfies the mass balance equation, and the desired deposition law. However, especially for heavy particles, the full reflection shows the full light beam characteristics and produces sometimes uneven, discontinuous particle distributions.

The model described in reference 8 uses the Slade depletion functions. The comparisons in this report are based on the Gaussian exponential depletion model in which

$$\dot{n}_x = \dot{n} e^{-\beta x/H}$$

which is the depletion function obtained for the perfect vertical mixing models described in the following sections.

#### A Differential Equation Diffusion Model

The anomalies identified with the Gaussian dispersion models, and also the anomalies in the closed form models are related to oversimplifications in the vertical direction.

In this section a model is presented in which the applicable diffusion equation is first solved in the vertical direction between the ground and the

inversion. The solution in terms of the crosswind integral as a function of time can then be turned into a dissemination solution.

The diffusion equation in which the diffusivity is nonconstant and in which the particles have gravitational settling is

$$\frac{\partial I}{\partial t} = K \frac{\partial^2 I}{\partial z^2} + \left( \frac{\partial K}{\partial z} + v_s \right) \frac{\partial I}{\partial z}$$

A physical model resulting in this diffusion equation is presented in appendix A. The diffusivity can be a function of  $z$  and  $t$ . Because very few problems with variable diffusivities can be solved in closed form, the solution was formulated in a finite difference form.

The determination of the diffusivity presented an anomaly. The solution of the differential equation for a point source in a field of uniform diffusivity is a Gaussian profile

$$I = \frac{\dot{n}}{u\sqrt{2\pi}\sigma_z} e^{-z^2/2\sigma_z^2}$$

where

$$\sigma_z = \sqrt{2Kt}$$

The Gaussian models use this distribution profile, but consistent with observations generally stipulate that the vertical dispersion grows linearly with time or distance rather than with the square root of time

$$\sigma_z = \theta_E x \quad \text{or} \quad \sigma_z = \theta_E ut$$

To obtain solutions from the differential equation, which use the same rate of growth of the parameters  $\sigma_z$ , the diffusivity was made a function of time.

If we require a dispersion  $\sigma_z = \theta_E ut$  and a rate of growth

$$\frac{d\sigma_z}{dt} = \theta_E u$$

then

$$\sigma_z \frac{d\sigma_z}{dt} = \theta^2 u^2 t$$

In a previous equation,  $\sigma_z \frac{d\sigma_z}{dt} = K$  so that the diffusivity in a vertical plane at the downwind distance  $x$  will be

$$K = \theta_E^2 u^2 t \quad \text{or} \quad K = \theta_E^2 ux$$

This assumption will give the diffusion model the same characteristics as the Gaussian models as long as the cloud can grow without constraints.

In modeling the convective layer the diffusivities should go to zero both at the ground and at the inversion. For the purposes of this study the following function was chosen for the diffusivity.

$$K_z = \theta^2 u^2 t \left[ \sin\left(\frac{\pi z}{H}\right) \right]^p$$

where  $p$  was arbitrarily chosen to be  $p = 0.1$  for most calculations.

#### The Perfect Vertical Mixing Model

When the turbulent mixing occurs rapidly, and the fall velocity of the particles is small, their distribution in the vertical direction very rapidly becomes uniform.

If perfect mixing in the vertical direction is assumed as an initial condition, simple closed form mathematical models can be derived which satisfy the requirement that the local deposition rate is the product of concentration and deposition velocity. Two idealized plume configurations have been treated, a vertical line source and a ground based point source. The vertical line source represents a good idealization for a fine plume which grows almost vertically and which gives off particles uniformly along its height. A ground-based point source represents a good idealization for a time plume in a high-wind in which the plume essentially remains attached to the ground. A simple model of a particle cloud from a continuously emitting source was created as shown in figure 6. The cloud has a rectangular cross section of height  $h$  and width  $\omega$  at a distance  $R$  downwind from the source.

To conserve the mass in the cloud, the sum of the particle flux through section B and the particle deposition in the element area  $\omega \Delta x$  must equal the influx of particles through section A.



If the particle concentration  $C$  is uniform and the deposition velocity is  $v_s$ , then the deposition rate in the element is

$$C v_s \omega \Delta C$$

The outflux of particles is

$$(C + \Delta C) (\omega + \Delta\omega) (h + \Delta h) u$$

and the influx of particles is

$$C \omega h u$$

This results in a differential equation for the concentration profile

$$\frac{dC}{dx} = -C \left( \frac{\beta}{h} + \frac{1}{h} \frac{dh}{dx} + \frac{1}{\omega} \frac{d\omega}{dx} \right)$$

where

$$\beta = v_s / u \text{ is the particle fall angle.}$$

If

$$\phi(x) = \left( \frac{\beta}{h} + \frac{1}{h} \frac{dh}{dx} + \frac{1}{\omega} \frac{d\omega}{dx} \right)$$

then the concentration profile is given by

$$C = C' e^{-\int \phi(x) dx}$$

If  $\dot{n}$  is the fiber flux at  $z_0$ , through a cloud  $h_0$ ,  $\omega_0$  then

$$C_0 h_0 \omega_0 u = \dot{n}$$

provides the input condition for the solution of the constant  $C'$ .

The vertical line source.- To model the vertical line source the height of a particle cloud is a constant  $H$ , and the width of the cloud is proportional to the radial distance. Therefore

$$h = H \quad \text{and} \quad \omega = \alpha x$$

and the expansion function is

$$\phi(x) = \beta/H + \frac{1}{x}$$

the concentration profile is

$$\begin{aligned} C &= C' e^{-\int \phi(x) dx} \\ &= C' e^{-\beta x/H - 1/x} \end{aligned}$$

The particle flux  $\dot{n}_0$  at  $x = x_0$  defines the initial condition so that

$$C_0 H x_0 u = \dot{n}_0$$

which gives

$$C = \frac{\dot{n}_0}{H \alpha u} \frac{1}{x} e^{-\beta x/H}$$

The exposure profile is the time integral of concentration

$$E = \int C dt$$

and since

$$N = \int \dot{n} dt$$

$$E = \frac{N}{H \alpha u} \frac{1}{x} e^{-\beta x/H}$$

The local ground deposition density is

$$D = E v_s$$

so that

$$D = \frac{N}{H\alpha x} e^{-\beta x/H}$$

This satisfies the condition that the total deposition must equal the number of particles

$$\int_0^{\infty} D \, dA = N$$

It is important to realize that the crosswind integral of concentration

$$I = \int C \, dy = \frac{\dot{n}}{uH} e^{-\beta x/H}$$

is independent of the lateral spreading of the cloud.

If, instead of assuming a uniform lateral concentration profile, we assume a Gaussian profile such that

$$C_{x,y} = C_{x,o} e^{-y^2/2\sigma_y^2}$$

whose crosswind integral is

$$I = C_{x,o} \sqrt{2\pi} \sigma_y$$

then

$$C_{x,o} = \frac{\dot{n}}{uH\sqrt{2\pi} \sigma_y} e^{-\beta x/H}$$

so that the concentration at any point is

$$C_{x,y} = \frac{\dot{n}}{\sqrt{2\pi} \sigma_y uH} e^{-\beta x/H} e^{-y^2/2\sigma_y^2}$$

and

$$E_{x,y} = \frac{N}{\sqrt{2\pi} \sigma_y uH} e^{-\beta x/H} e^{-y^2/2\sigma_y^2}$$

The ground-based point source.- To model a ground-based point source the height of the cloud is assumed zero at the source. If we assume the height to vary as

$$h = H(1 - e^{-\gamma x/H})$$

and

$$\omega = \alpha x$$

We get a rectangular cloud growing from a point on the ground for which the expansion function

$$\phi(x) = \frac{\beta}{H(1 - e^{-\gamma x/H})} + \frac{\gamma e^{-\gamma x/H}}{H(1 - e^{-\gamma x/H})} + \frac{1}{x}$$

To simplify the expressions we substitute

$$e^{-\gamma x/H} = \tau$$

The concentration profile is

$$C = \frac{\dot{n}_o}{\alpha H u x} \left( \frac{1 - \tau_o}{\tau_o} \right)^{\beta/\gamma} \left( \frac{1}{1 - \tau} \right) \left( \frac{\tau}{1 - \tau} \right)^{\beta/\gamma}$$

and the exposure profile is

$$E = \frac{N}{\alpha Hu x} \left( \frac{1 - \tau_o}{\tau_o} \right)^{\beta/\gamma} \left( \frac{1}{1 - \tau} \right) \left( \frac{\tau}{1 - \tau} \right)^{\beta/\gamma}$$

and the crosswind concentration integral

$$I_x = \frac{N}{Hu} \left( \frac{1 - \tau_o}{\tau_o} \right)^{\beta/\gamma} \left( \frac{1}{1 - \tau} \right) \left( \frac{\tau}{1 - \tau} \right)^{\beta/\gamma}$$

If the crosswind concentration profile is Gaussian

$$C_{x,y} = \frac{\dot{n}}{\sqrt{2\pi} \sigma_y Hu} \left( \frac{1 - \tau_o}{\tau_o} \right)^{\beta/\gamma} \left( \frac{1}{1 - \tau} \right) \left( \frac{\tau}{1 - \tau} \right)^{\beta/\gamma} e^{-y^2/2\sigma_y^2}$$

where again  $\sigma_y$ , the lateral dispersion can be chosen to fit the dissemination data.

Most frequently, predictions from the diffusion models are required in the form of contours of (constant) exposure.

The equation for the distance  $y$  of the contour 'E' from the centerline of calculations is

$$y^2 = 2\sigma_y^2 \left\{ \ln \left( \frac{N}{\sqrt{2} \sigma_y Hu} \right) + \frac{\beta}{\gamma} \left[ \ln \left( \frac{1 - \tau_o}{\tau_o} \right) + \ln \left( \frac{\tau}{1 - \tau} \right) \right] - \ln(1 - z) - \ln E \right\}$$

Figure 6 shows a contour plot for the release conditions assumed for neutral atmospheres.

$$\begin{aligned} N &= 10^9 & H &= 400 \text{ m} \\ v_s &= 0.02 \text{ m/s} & u &= 6 \text{ m/s} \\ \theta_E &= 0.07 & \text{and } \gamma &= \theta_E \times \sqrt{\frac{\pi}{2}} \\ \theta_A &= 0.07 & \sigma_y &= x\theta_A \\ \gamma &= 0.0877 \end{aligned}$$

## MODEL COMPARISONS

### Elevated Sources

Four models have been presented in the previous sections. They are the Gaussian partial reflection model, the Gaussian exponential depletion model, the perfect vertical-mixing models, and the analytical diffusion model.

These four models will be compared in this section. All models have identical spreading in the transverse or crosswind direction because the almost linearly growing Gaussian dispersion represents the only existing data, and has been incorporated in all models. The comparisons are, therefore, made in terms of crosswind integrals.

All four models were used to calculate the crosswind integrals for ten downwind sections and all points between the ground and the inversion.

These calculations were made for two particle fall velocities, 0.02 m/s and 0.2 m/s in three meteorological conditions.

Table I shows a matrix of model parameters for three meteorological conditions.

TABLE I.- MODEL PARAMETERS

| Condition | Inversion height, H | Wind vel., u | Vert. disp. angle, $\theta_E$ |
|-----------|---------------------|--------------|-------------------------------|
| Stable    | 100                 | 1.5          | 0.025                         |
| Neutral   | 400                 | 6.0          | 0.07                          |
| Unstable  | 1000                | 2.0          | 0.15                          |

The results for the vertical particle distribution are plotted as isometric views of the crosswind integrals at ten downwind stations in figures 8 to 13.

Table II shows the matrix of conditions applicable to each of these figures.

TABLE II.- MODEL INPUT CONDITIONS

| Meteorological category | Particle velocity m/s | Isometric figure | Ground-level figure |
|-------------------------|-----------------------|------------------|---------------------|
| Stable                  | 0.02                  | 8                | 14                  |
| Stable                  | 0.2                   | 9                | 15                  |
| Neutral                 | 0.02                  | 10               | 16                  |
| Neutral                 | 0.2                   | 11               | 17                  |
| Unstable                | 0.02                  | 12               | 18                  |
| Unstable                | 0.2                   | 13               | 19                  |

While figures 8 through 13 show the distribution of the particles in the vertical and downwind directions, a more precise comparison of the models is presented in figures 14 through 19. They are semilogarithmic representations of the ground-level values of the crosswind integrals.

The isometric sections show that in five of the six conditions, the turbulence is strong enough to produce essentially perfect vertical mixing.

The isometric sections show that in neutral and unstable weather (figs. 9 through 12) the vertical distribution becomes uniform before significant depletion occurs, even for the high fall velocity. In the stable atmosphere and the 2 cm/s fall velocity the distribution becomes triangular (fig. 8) at the 2000 m range, and for the 20 cm/s fall velocity (fig. 9) the cloud falls to the ground before dispersing significantly.

The ratio of dispersion angle  $\theta_E$  to the fall angle  $\beta$  is the logical measure of the dispersive strength. From these six cases we obtain the result that the cloud will fall to the ground if  $\theta_E/\beta < 1$ , and that it will deplete after distributing uniformly if  $\theta_E/\beta > 2$ .

The semilogarithmic presentation of the ground-level values of the crosswind integrals show the smaller differences between the four models in detail. Figure 14 shows the solutions for the 2 cm/s fall velocity particles in the stable atmosphere. The straight solid line is the result for the perfect vertical-mixing model. The Gaussian exponential depletion model rapidly approaches this solution. The analytical diffusion model also asymptotically approaches this solution. Only the Gaussian partial reflection model which was tuned to agree with the analytical diffusion model 2000 m downwind from the source deviates from the other model results. This trend agrees with the analytical observation that the mathematical form of the deposition by partial

reflection does not agree with the constant fall velocity deposition. The same trend is visible for the other atmospheric conditions, especially in figures 15, 16 and 19. In all cases, the reflection coefficients had been determined by iteration so that the Gaussian partial reflection model would agree with the analytical diffusion model at or just beyond the peak values of the crosswind integral. Table III lists the values of the partial reflection coefficients used in the six analyses.

TABLE III.- PARTIAL REFLECTION COEFFICIENTS

| Condition | Light part.<br>2 cm/s | Heavy partic.<br>20 cm/s |
|-----------|-----------------------|--------------------------|
| Stable    | r = 0.5               | r = 0.01                 |
| Neutral   | 0.85                  | 0.45                     |
| Unstable  | 0.9                   | 0.35                     |

While the use of the partial reflection coefficient allows tuning the model for a good agreement at one distance, it is important to realize that, at long distances downwind, the model will predict conservative values of contamination.

The Gaussian exponential depletion model in all cases predicted the highest peak values and converged to the solution of the perfect vertical mixing model. In the stable atmosphere with the heavy particles this solution (fig. 15) breaks down. It converges to the solution for the perfect vertical mixing model, although because of the low turbulence, this weather situation never produces perfect vertical mixing for such heavy particles (fig. 9). Also, the bouncing light beam effect is very visible in this solution. Notwithstanding those shortcomings, the solutions predict the correct maximum values, and the errors only become large when the exposures are very much lower than the maxima observed.

#### Ground-Based Point Sources

The perfect vertical mixing model with the ground-based point source has been compared to the solutions obtained from the diffusion model. The elevation growth angle of the cloud  $\gamma$  was assumed to be equal to the elevation dispersion angle  $\theta_E \times \sqrt{\pi/2}$  to match the maxima of the original Gaussian and uniform distributions.



Figure 20 shows the semilogarithmic presentation of the ground-level values of the crosswind integral. The two models agree closely over the 10 km range. Similarly, good agreement was obtained for neutral atmospheres (fig. 21) and the unstable atmosphere (fig. 22). The ground-based point source model has the great advantage that contamination levels can be computed from a single closed-form algebraic expression, while the Gaussian models contain series of terms from successive reflections, and the diffusion model requires a slow numerical solution of its differential equation.

#### CONCLUDING REMARKS

The Gaussian dissemination models which were used in the carbon fiber risk assessment, have been compared to an analytical diffusion model. Partial reflection coefficients were obtained for pollutant particles of 2 cm/s and 20 cm/s fall velocities, characteristic for single carbon fibers and small clumps. The model predictions based on these reflection coefficients were in close agreement with the solutions from the diffusion model for similar atmospheric conditions. For large downwind distances the Gaussian models tended to predict higher than expected exposures. For the graphite fiber risk assessment, the use of these Gaussian models is expected to provide reliable, if somewhat conservative, exposure calculations.

Because most pollutant cloud models showed that uniform vertical mixing over the convective air layers was reached very rapidly, a perfect vertical mixing model was established which is useful for fast and simple exposure calculations. Those models provided a parametric analysis technique for the graphite risk assessment.

## APPENDIX A

### DIMENSIONAL CONDENSATION OF THE DIFFUSION PROBLEM

For a continuous particle source, the concentration of particles in a cell drifting with the wind can be expressed by a two-dimensional diffusion equation

$$\frac{\partial C}{\partial t} = K_y \frac{\partial^2 C}{\partial y^2} + \frac{\partial C}{\partial z} \left( \frac{\partial K_z}{\partial z} + v_s \right) + K_z \frac{\partial^2 C}{\partial z^2} \quad (1)$$

There are some solution types for this equation which have the form

$$C = C' F_1(y, t) F_2(z, t) \quad (2)$$

in which the functions of  $y$  and  $z$  are separable. If the function describing the distribution of the particles in the crosswind direction,  $F_1(y, t)$ , has the characteristics of a distribution function, such that its integral in the  $y$  direction is a constant,

$$\int_{-\infty}^{\infty} F_1(y, t) dy = B \quad (3)$$

then the two-dimensional diffusion problem can be condensed into a one-dimensional problem in the vertical direction.

The various differentials of the concentration profile are

$$\frac{\partial C}{\partial t} = C' F_1(y, t) \frac{\partial}{\partial t} F_2(z, t) + C' F_2(z, t) \frac{\partial}{\partial t} F_1(y, t)$$

$$\frac{\partial C}{\partial z} = C' F_1(y, t) \frac{\partial}{\partial z} F_2(z, t)$$

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$$\frac{\partial^2 C}{\partial z^2} = C' F_1(y, t) \frac{\partial^2}{\partial z^2} F_2(z, t)$$

$$\frac{\partial^2 C}{\partial y^2} = C' F_2(z, t) \frac{\partial^2}{\partial y^2} F_1(y, t)$$

When these are substituted into equation (1)

$$\begin{aligned} F_1(y, t) \frac{\partial}{\partial t} F_2(z, t) + F_2(z, t) \frac{\partial}{\partial t} F_1(y, t) &= K F_1(y, t) \frac{\partial^2}{\partial z^2} F_2(z, t) \\ &+ F_1(y, t) \frac{\partial}{\partial z} F_2(z, t) \left( \frac{\partial K}{\partial z} + v_s \right) \\ &+ K F_2(z, t) \frac{\partial^2}{\partial y^2} F_1(y, t) \end{aligned} \quad (4)$$

If this equation is integrated with respect to  $y$

$$\begin{aligned} \frac{\partial}{\partial t} F_2(z, t) \int_{-\infty}^{\infty} F_1(y, t) dy + F_2(z, t) \int_{-\infty}^{\infty} \frac{\partial}{\partial t} F_1(y, t) dy &= K \frac{\partial^2}{\partial z^2} F_2(z, t) \\ &\times \int_{-\infty}^{\infty} F_1(y, t) dy + \left( \frac{\partial K}{\partial z} + v_s \right) \frac{\partial}{\partial z} F_2(z, t) \\ &\times \int_{-\infty}^{\infty} F_1(y, t) dy + K F_2(z, t) \int_{-\infty}^{\infty} \frac{\partial^2}{\partial y^2} F_1(y, t) dy \end{aligned} \quad (5)$$

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Since  $F_1(y,t)$  is a distribution function which has

$$\int_{-\infty}^{\infty} F_1(y,t) dy = B$$

then

$$\int_{-\infty}^{\infty} \frac{\partial}{\partial t} F_1(y,t) dy = \int_{-\infty}^{\infty} \frac{\partial^2}{\partial y^2} F_1(y,t) dy = 0$$

When these are substituted in equation (5), we get

$$B \frac{\partial}{\partial t} F_2(z,t) = BK \frac{\partial^2}{\partial z^2} F_2(z,t) + B \left( \frac{\partial K}{\partial z} + v_s \right) \frac{\partial}{\partial z} F_2(z,t) \quad (6)$$

If  $I$  is defined as the crosswind integral of concentration

$$I = C' F_2(z,t) \int_{-\infty}^{\infty} F_1(y,t) dy$$

Then, equation (6) becomes

$$\frac{\partial}{\partial t} I = K \frac{\partial^2}{\partial z^2} I + \left( \frac{\partial K}{\partial z} + v_s \right) \frac{\partial I}{\partial z} \quad (7)$$

This is a one-dimensional diffusion problem in the vertical direction. The dissemination models derived herein are first obtained in terms of the crosswind integral. Any lateral distribution such as the Gaussian can be given to the crosswise concentration profile.

## APPENDIX B

### A PHYSICAL MODEL FOR THE DIFFUSION EQUATION

The atmosphere can be subdivided into a series of layers. Perfect mixing can be assumed within each layer together with a fixed air exchange between adjacent layers.

Figure 23 shows a series of five layers of depth  $\epsilon$  and lateral dimensions  $\Delta x$  and  $\Delta y$ . The layers are joined by imaginary airflow ducts exchanging air at a flow rates  $q$ . Simultaneously, the particles can fall through the layers at a fall velocity  $v_s$ .

Let the concentration around the center element be described by the Taylor expansion

$$C(\epsilon) = C_o + \frac{\partial C}{\partial z} \epsilon + \frac{1}{2} \epsilon^2 \frac{\partial^2 C}{\partial z^2}$$

and let the flow rates  $q$  also be expressed as

$$q(\epsilon) = q_o + \frac{\partial q}{\partial z} \epsilon + \frac{\epsilon^2}{2} \frac{\partial^2 q}{\partial z^2}$$

If the concentration  $C_{+1}$  is defined as  $C(\epsilon)$  then

$$C(\epsilon) = C_{+1} = C_o + \epsilon \frac{\partial C}{\partial z} + \frac{\epsilon^2}{2} \frac{\partial^2 C}{\partial z^2}$$

and if the exchange flow between  $C_o$  and  $C_{+1}$  is defined as

$$q(\epsilon/2) = q_{o,1} = q_o + \frac{\epsilon}{2} \frac{\partial q}{\partial z} + \frac{\epsilon^2}{8} \frac{\partial^2 q}{\partial z^2}$$

The particle flow  $\Delta N$  into the center element is then

$$\Delta N = \Delta t \left\{ q_{o,1} (C_{+1} - C_o) + q_{o,-1} (C_{-1} - C_o) \right\}$$

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The settlement flow through the boundary is

$$\Delta t \left\{ v_s \Delta x \Delta y (C_{+1} - C_0) \right\}$$

After expanding concentrations and flow rates

$$\Delta N = \Delta t \left\{ q_0 \epsilon^2 \frac{\partial^2 C}{\partial z^2} + \epsilon^2 \frac{\partial q}{\partial z} \frac{\partial C}{\partial z} + v_s \Delta x \Delta y \epsilon \frac{\partial C}{\partial z} \right\}$$

if we define an exchange flow velocity  $v_a$  such that

$$v_a \Delta x \Delta y = q$$

then

$$\frac{\Delta N}{\Delta t \Delta x \Delta y} = v_a \epsilon \frac{\partial^2 C}{\partial z^2} + \frac{\partial v_a \epsilon}{\partial z} \frac{\partial C}{\partial z} + v_s \frac{\partial C}{\partial z}$$

If the product of layer height and exchange flow velocity is  $K = v_a \epsilon$ , then this equation reduces to the normal diffusion equation

$$\frac{\partial C}{\partial t} = K \frac{\partial^2 C}{\partial z^2} + \frac{\partial K}{\partial z} \frac{\partial C}{\partial z} + v_s \frac{\partial C}{\partial z}$$

The finite element formulation for this equation is

$$\frac{\Delta C}{\Delta t} = \left\{ \frac{K \epsilon/2}{\epsilon^2} + \frac{v_s}{\epsilon} \right\} (C_{+1} - C_0) + \frac{K - \epsilon/2}{\epsilon^2} (C_{-1} - C_0)$$

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For the outer layers the equation will be at the upper bound

$$\frac{\Delta C}{\Delta t} = -\frac{v_s}{\epsilon} C_0 + \frac{K_{-\epsilon/2}}{\epsilon^2} (C_{-1} - C_0)$$

and for the lower bound

$$\frac{\Delta C}{\Delta t} = \left\{ \frac{v_s}{\epsilon} + \frac{K_{\epsilon/2}}{\epsilon^2} \right\} (C_{+1} - C_0)$$

Those formulations provide mass-conservative solutions to the one-dimensional diffusion problem.

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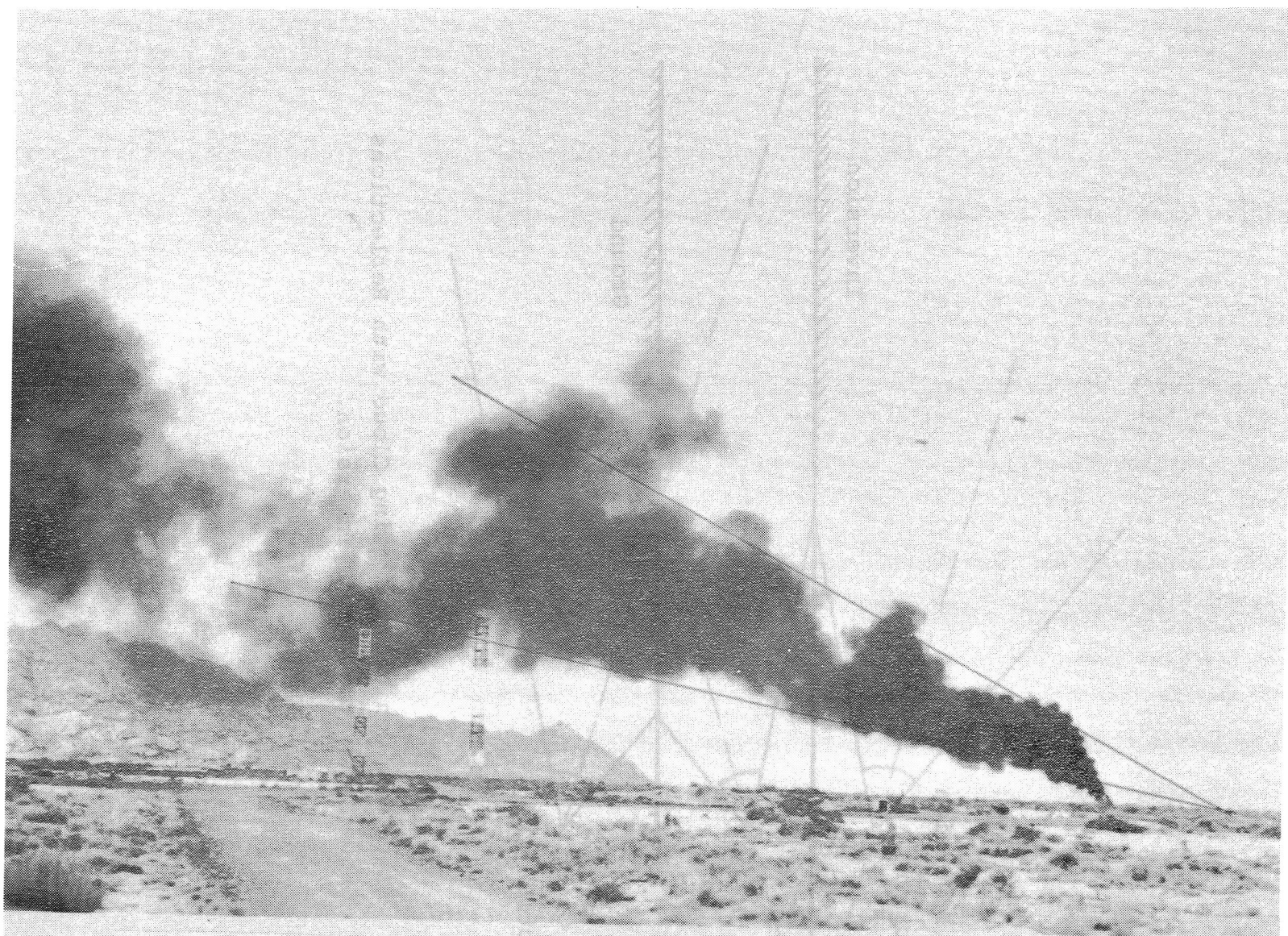


Figure 1. Typical Fuel Fire Plume and Conical Expansion Envelope

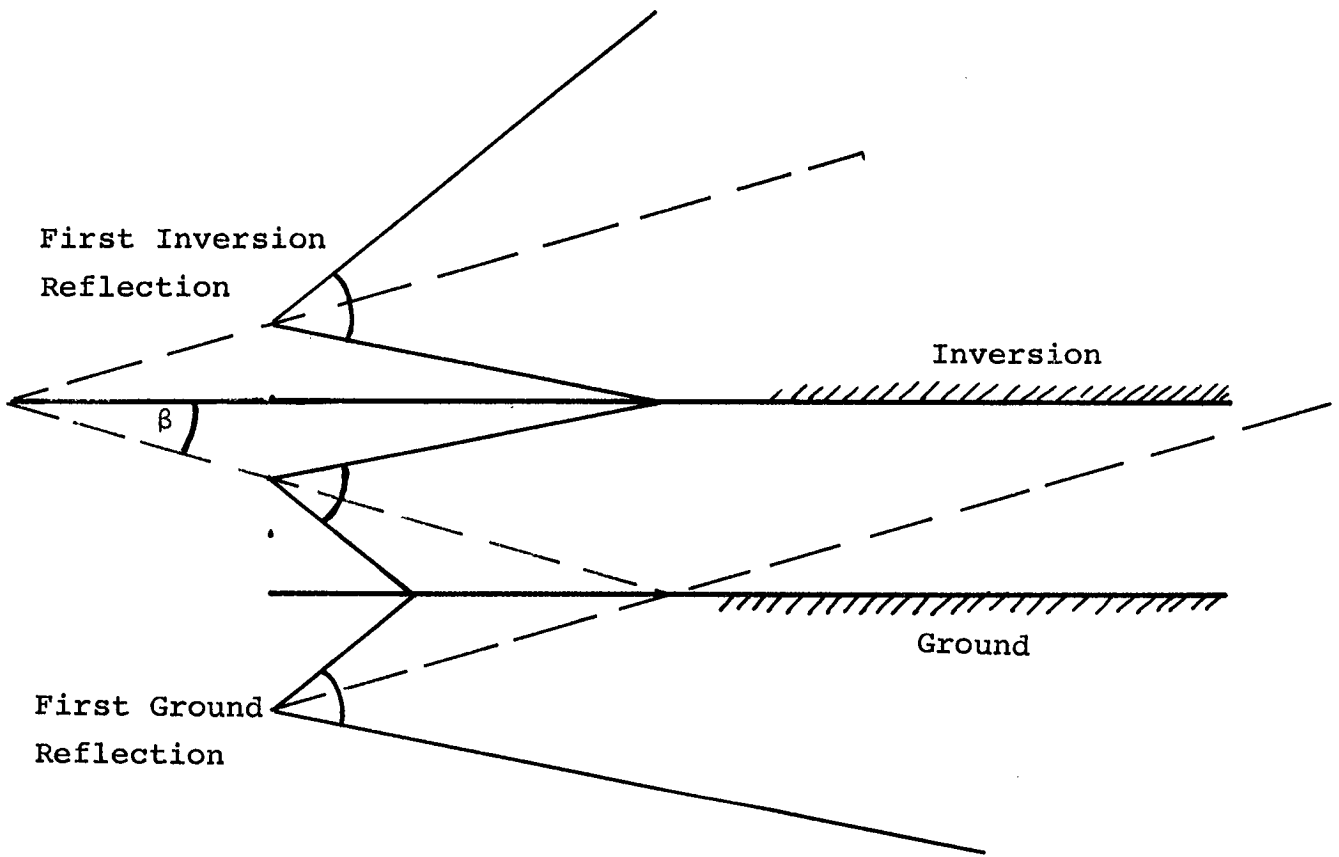


Figure 2. Conically Growing Cloud with Reflections Ground and Atmospheric Inversion.

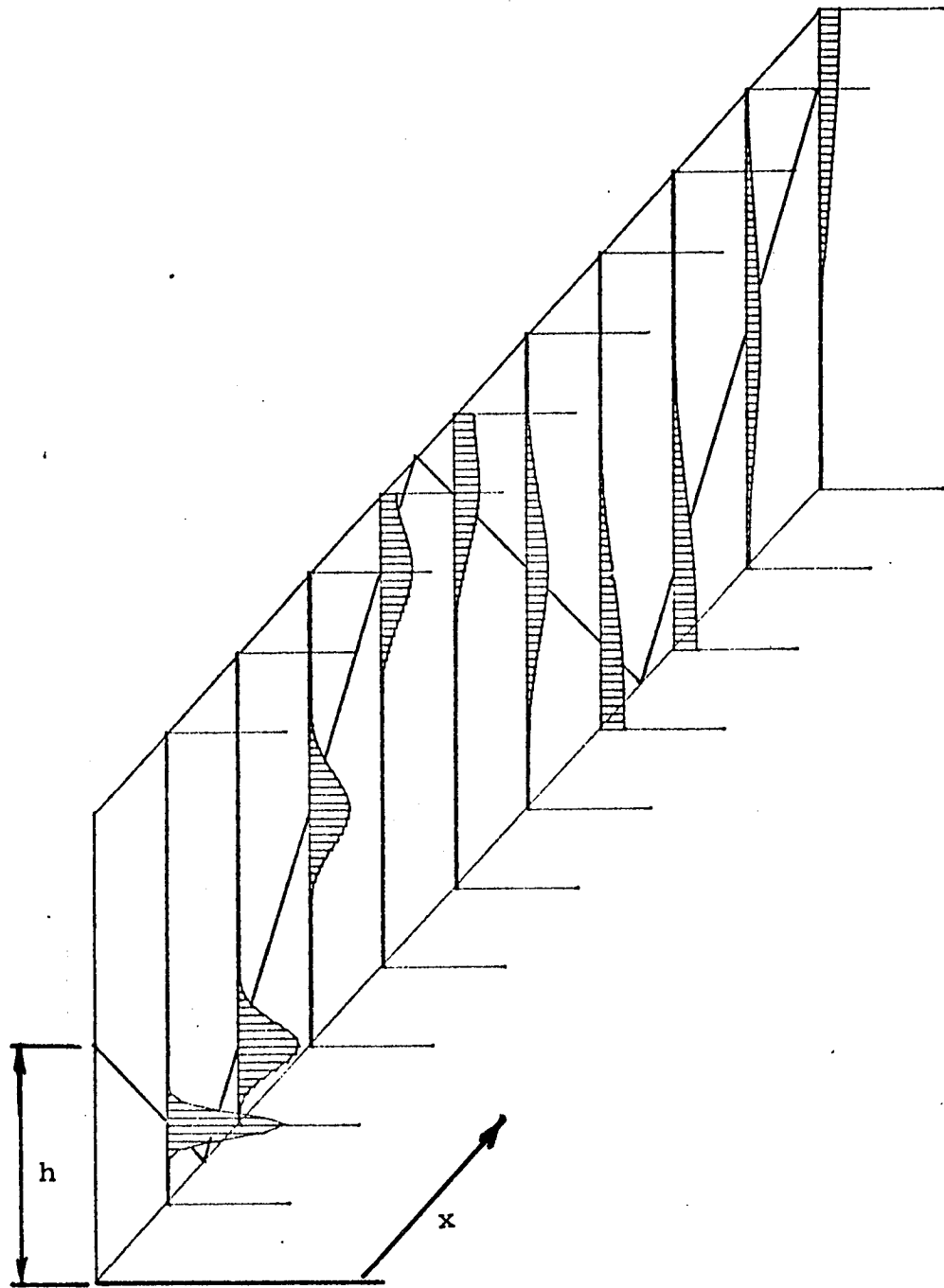


Figure 3. Perfect Reflection of a Slow-Growing Cloud.

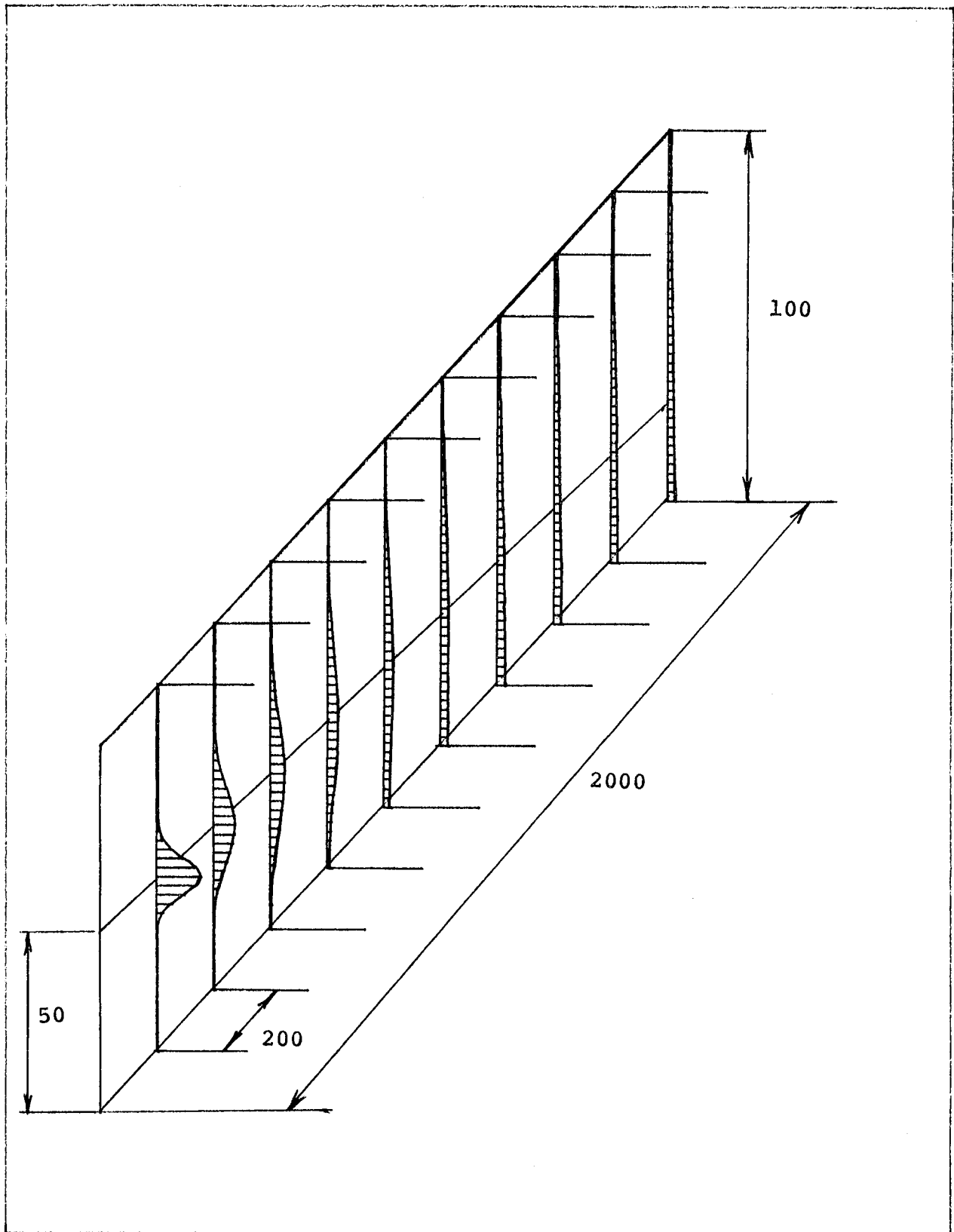


Figure 4. Cross-wind Concentration Integrals in Stable Atmosphere over 2000m Range.

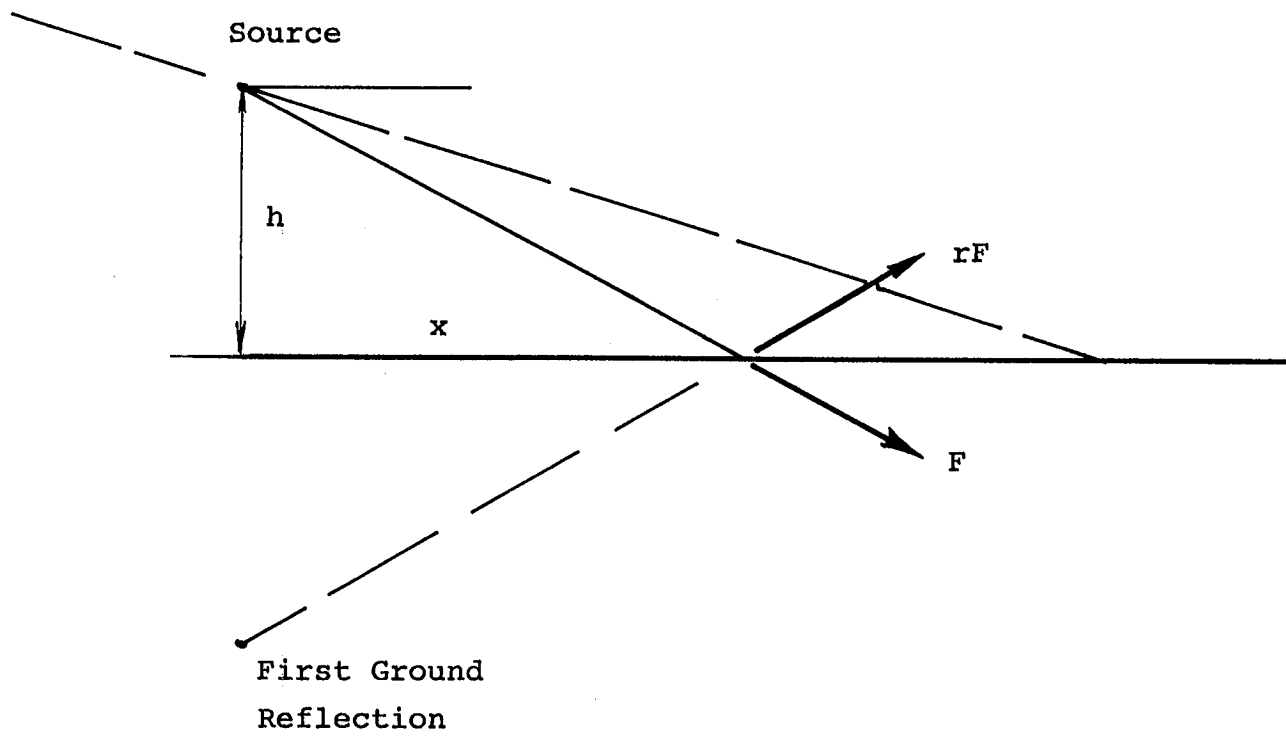


Figure 5. Definition of the Flux Vector

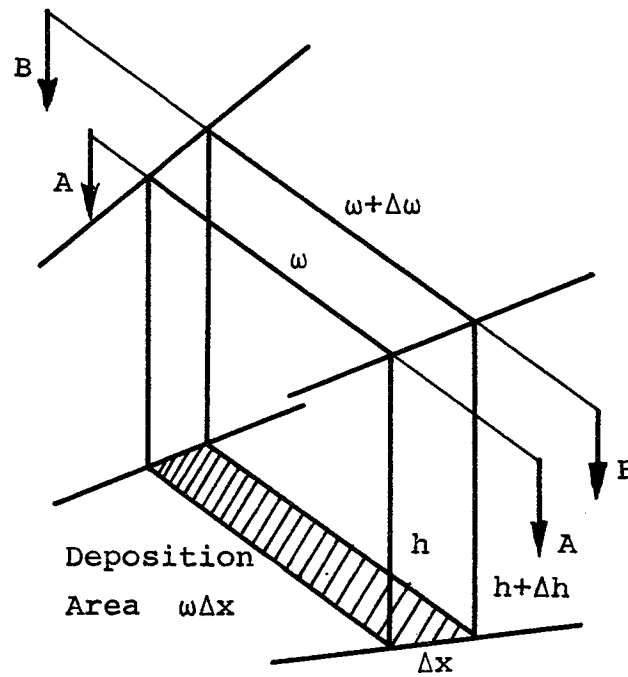


Figure 6. Configuration of a Typical Section Through an Expanding Rectangular Cloud.

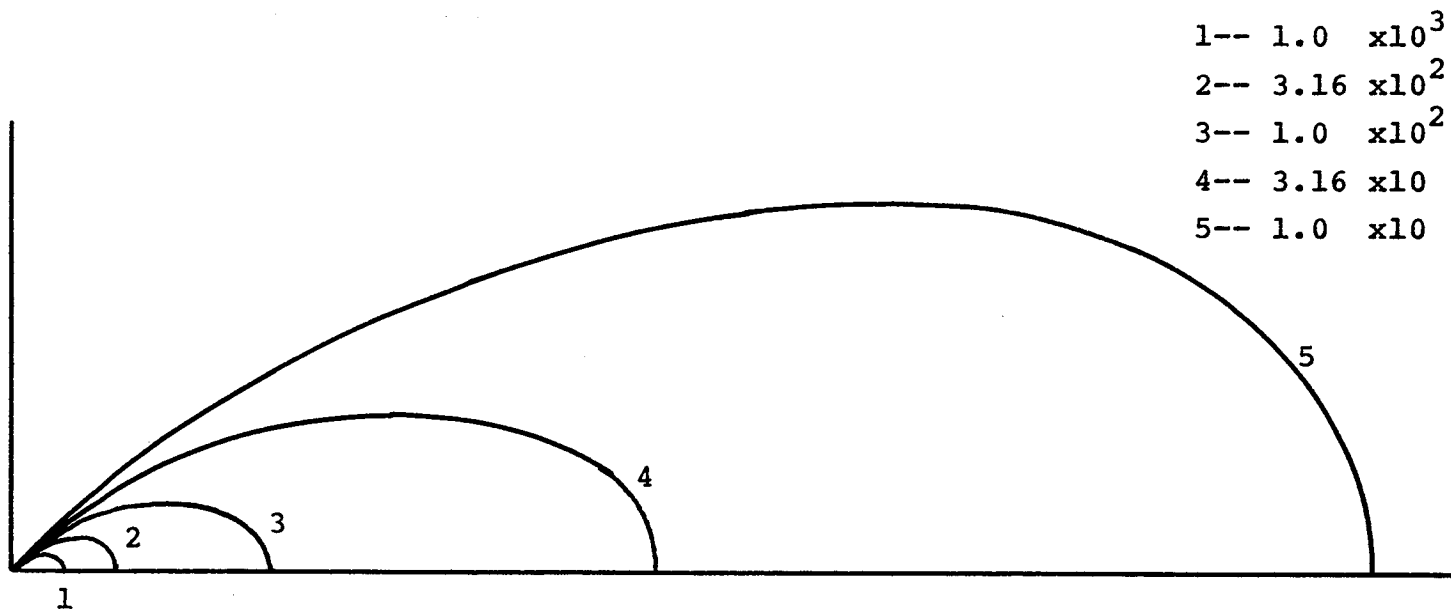
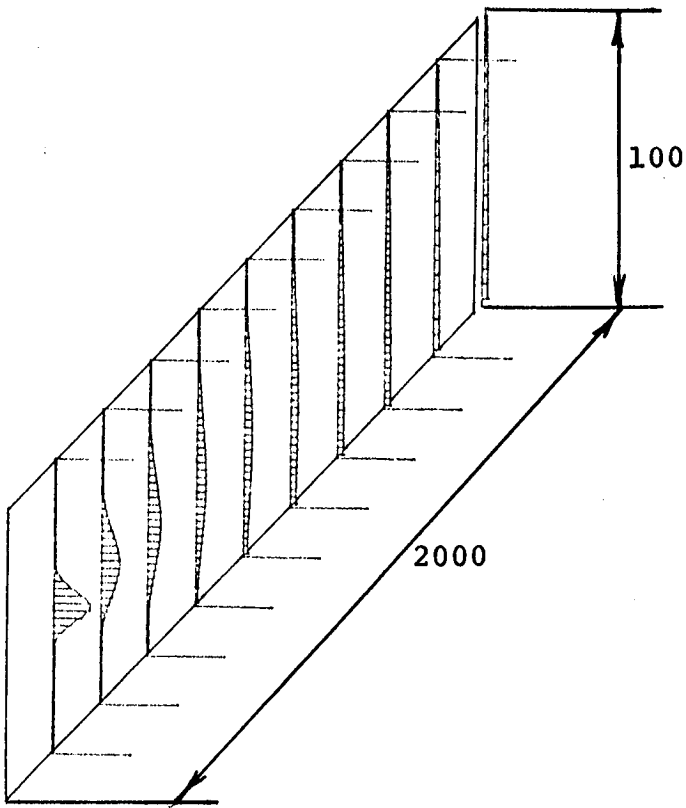
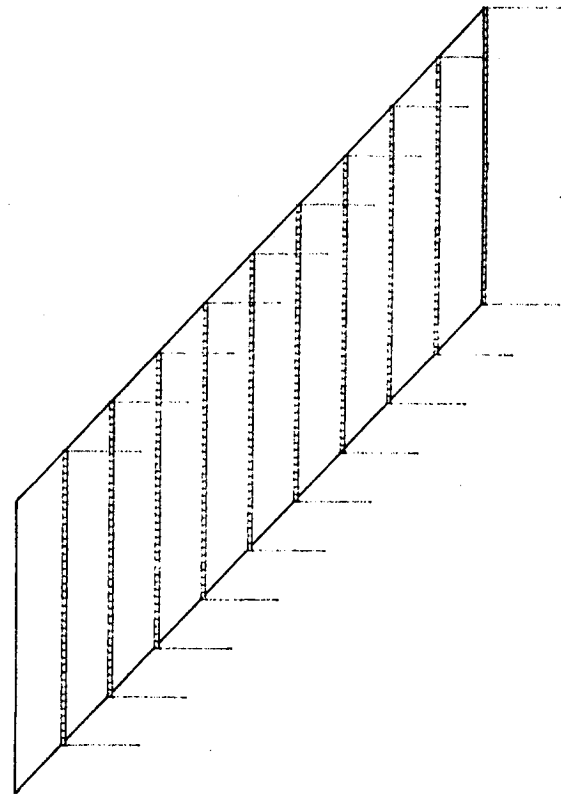


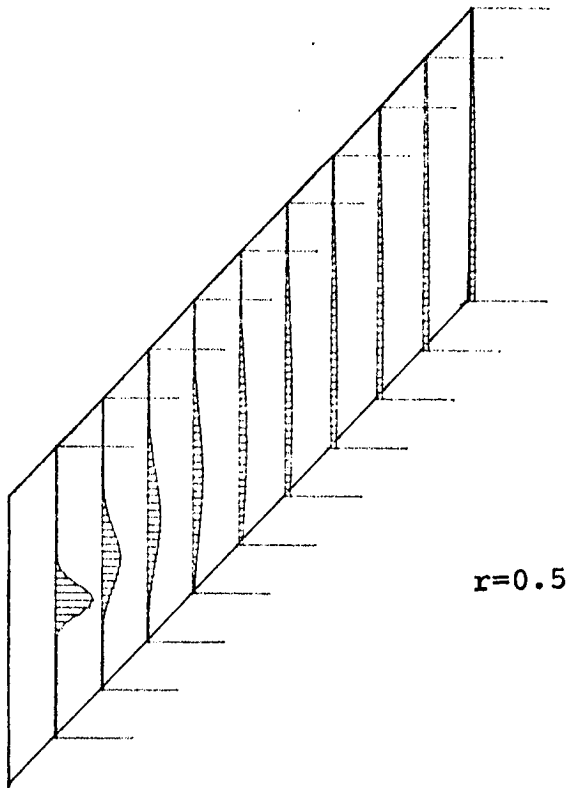
Figure 7. Exposure Contours for Ground-Based Point Source  
in Neutral Atmosphere for Release of  $10^9$  Particles.



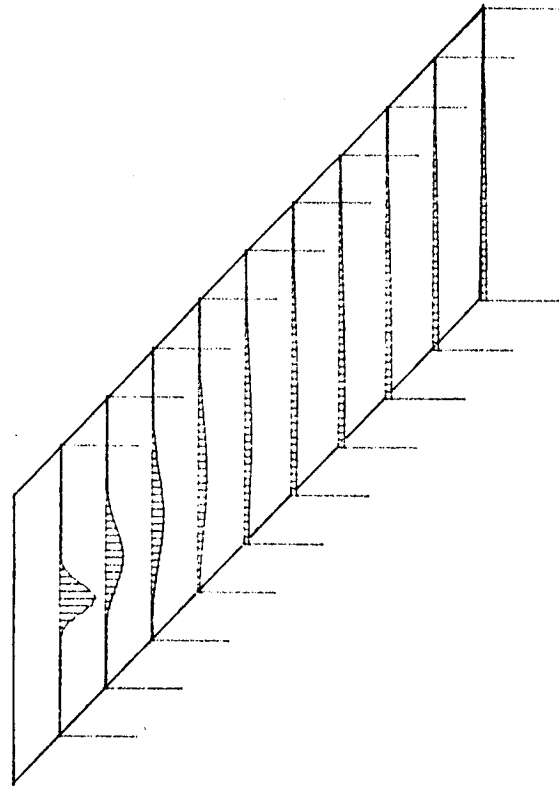
a) Diffusion Model



b) Perfect Vertical Mixing Model,  
Line Source



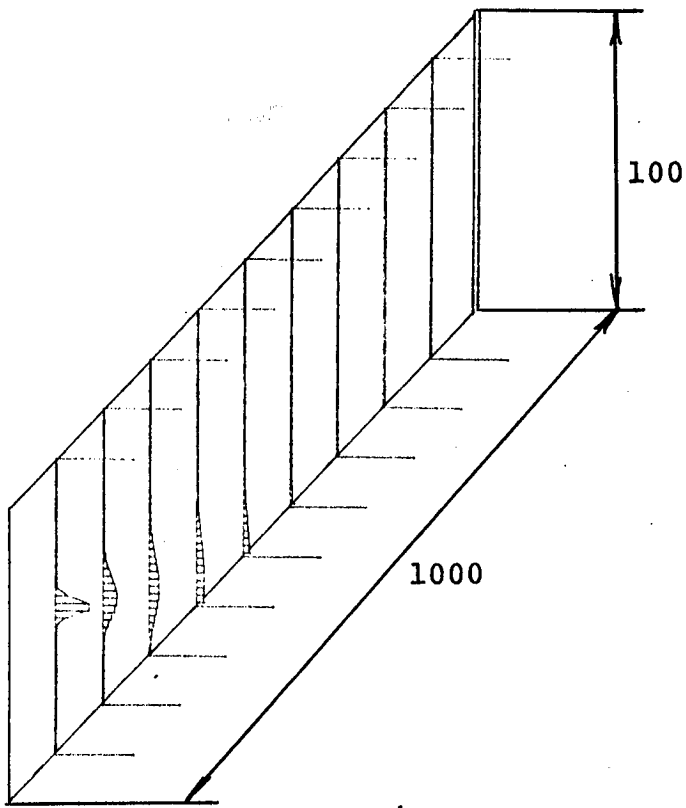
c) Gaussian Partial Reflection Model



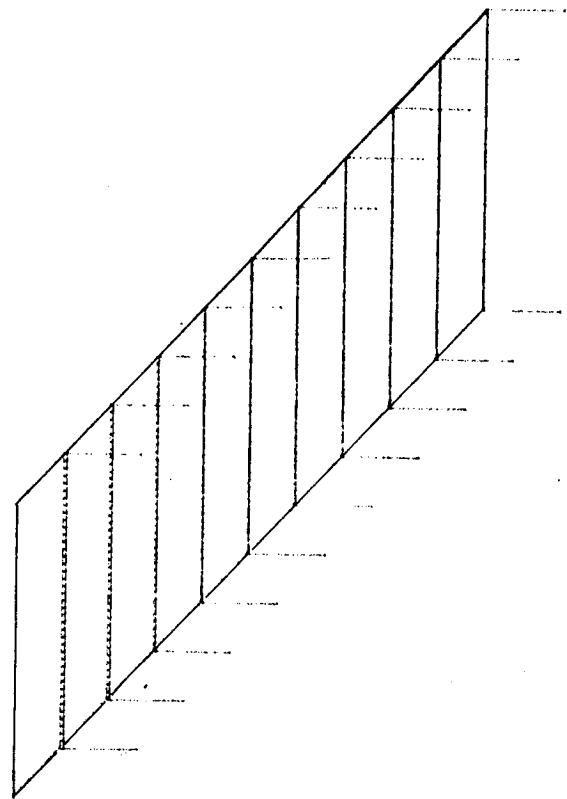
d) Gaussian Exponential Depletion Model

Figure 8. Predicted Crosswind Integrals for Stable Atmosphere -  $v_s = 0.02$  m/s

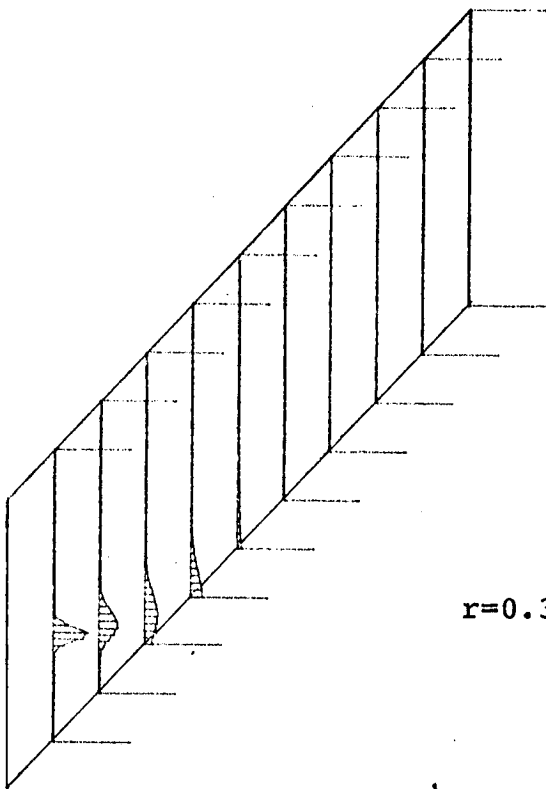




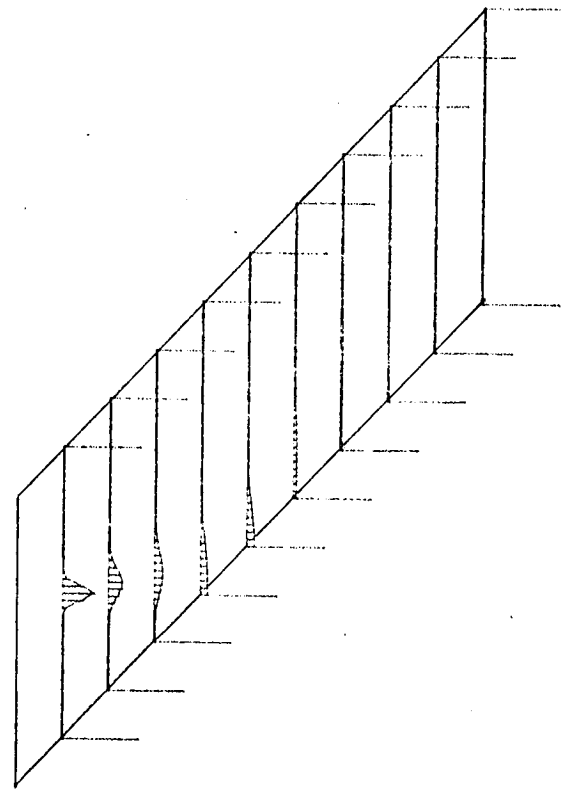
a) Diffusion Model



b) Perfect Vertical Mixing Model,  
Line Source



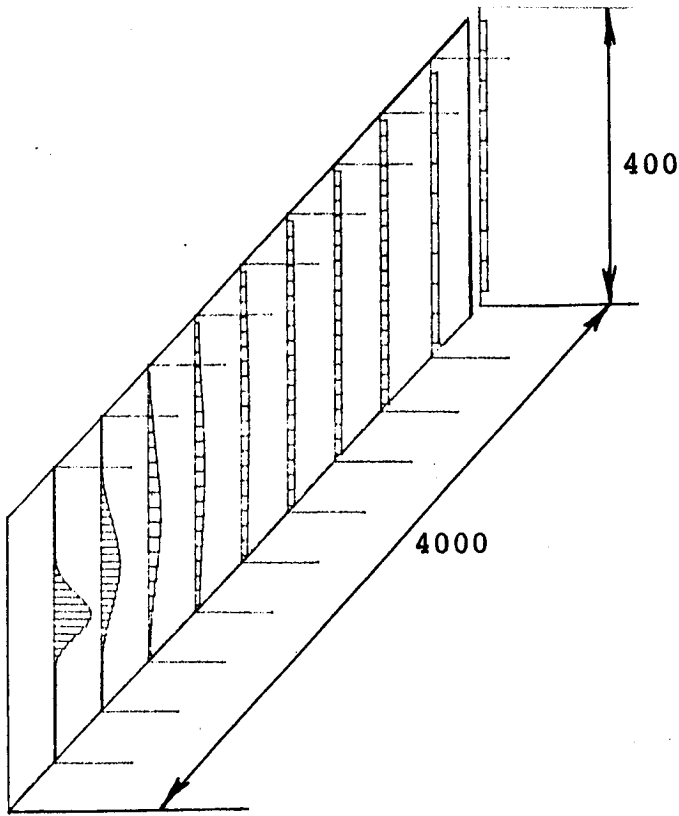
c) Gaussian Partial Reflection Model



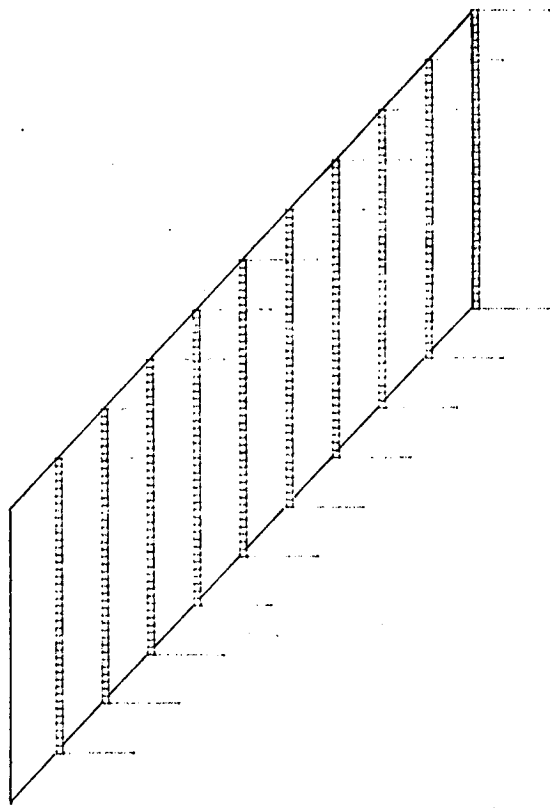
d) Gaussian Exponential Depletion Model

Figure 9. Predicted Crosswind Integrals for Stable Atmospheres -

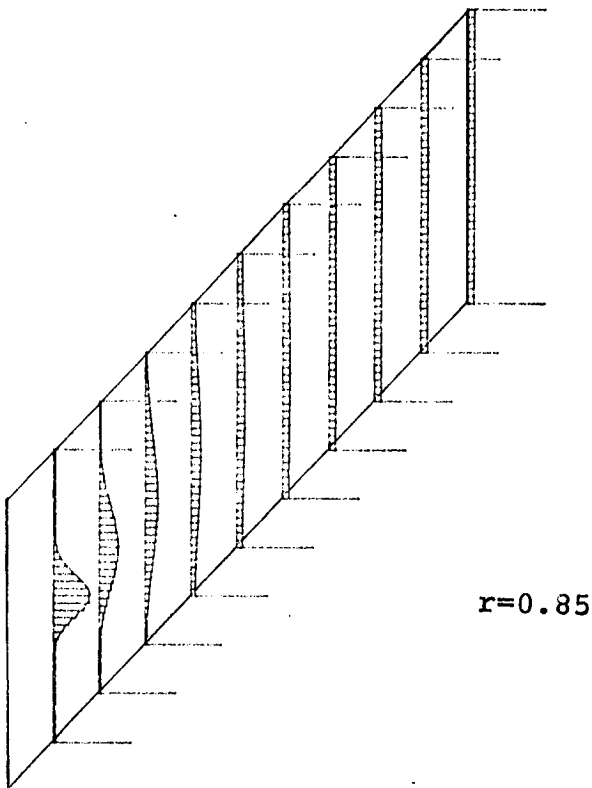
$$v_s = 0.2 \text{ m/s}$$



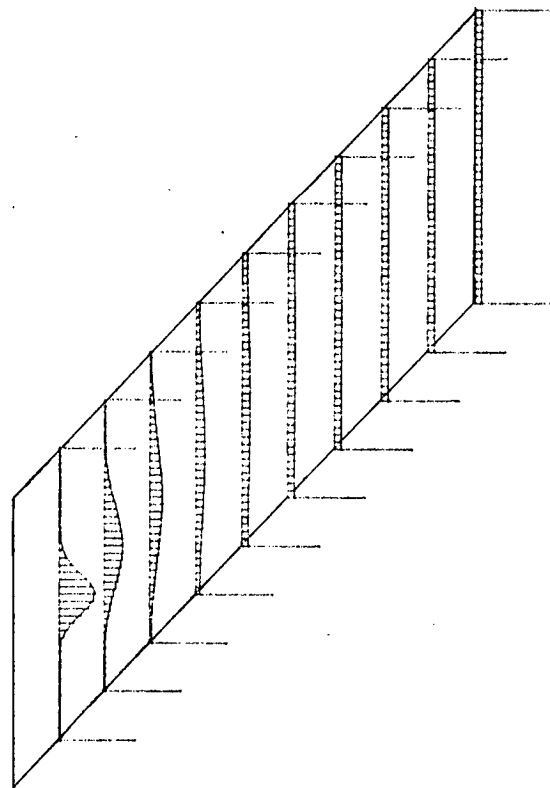
a) Diffusion Model



b) Perfect Vertical Mixing Model,  
Line Source



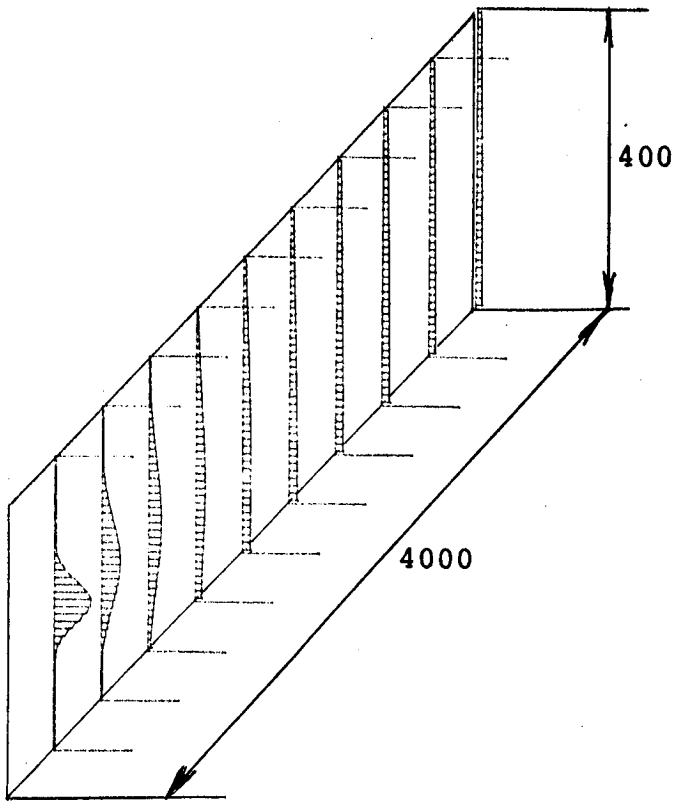
c) Gaussian Partial Reflection Model



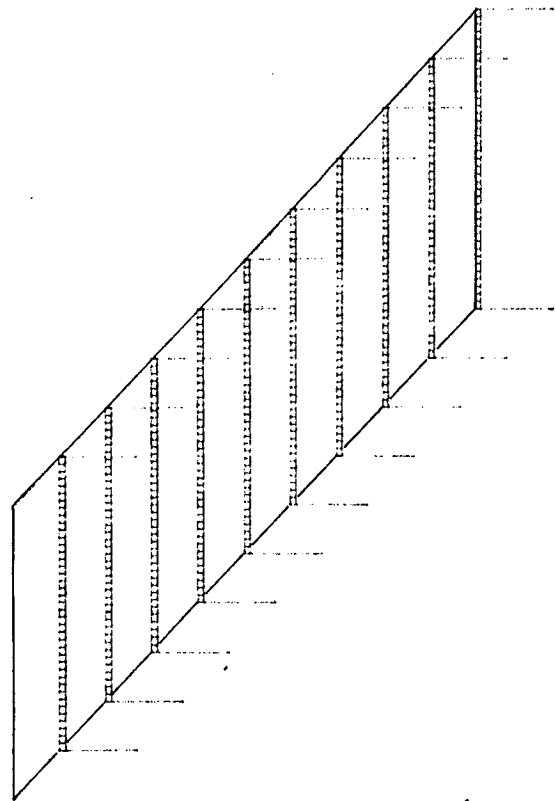
d) Gaussian Exponential Depletion Model

Figure 10. Predicted Crosswind Integrals for Neutral Atmosphere

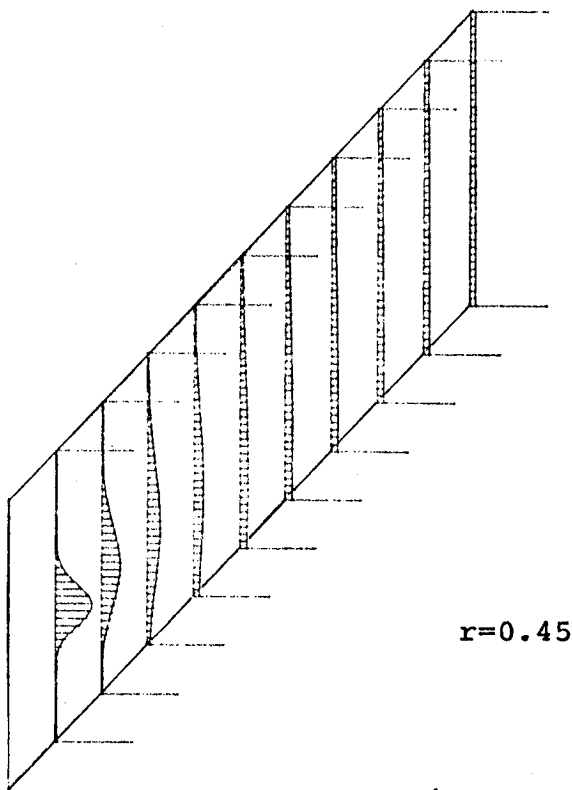
$$v_s = 0.02 \text{ m/s}$$



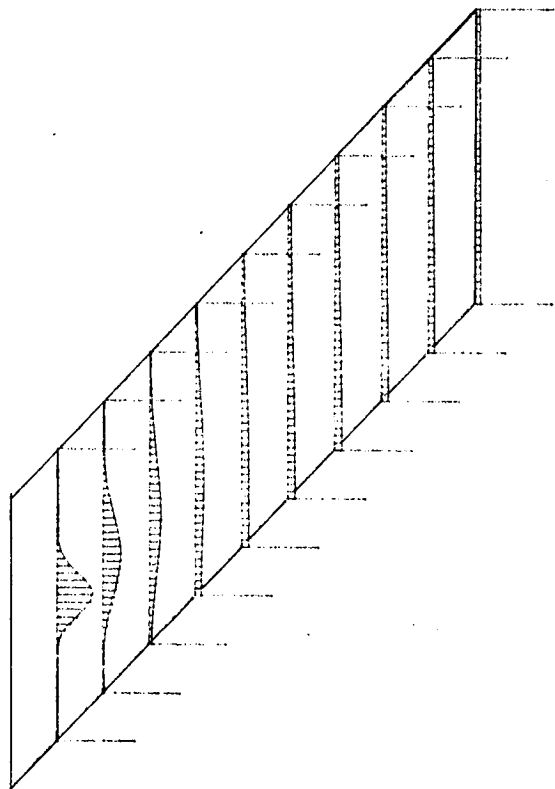
a) Diffusion Model



b) Perfect Vertical Mixing Model,  
Line Source

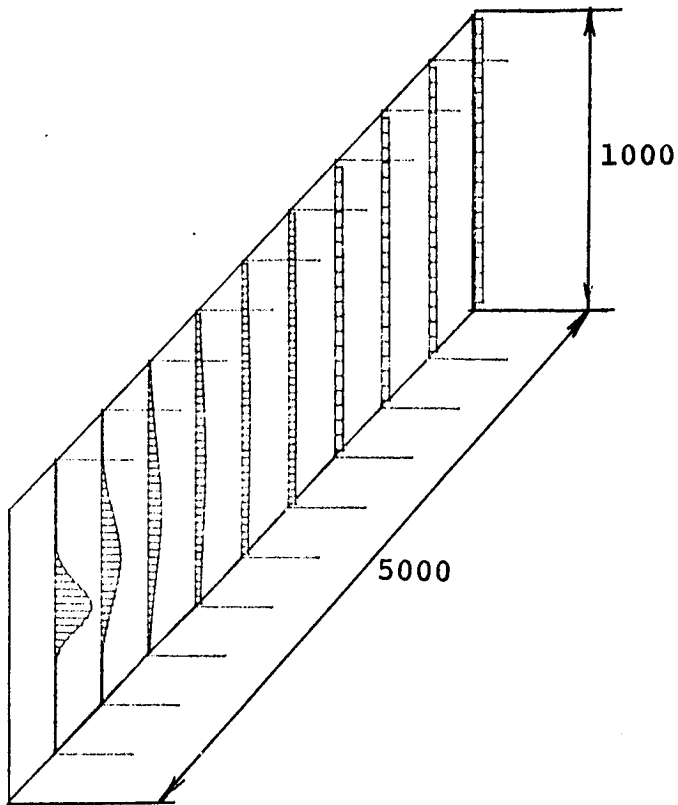


c) Gaussian Partial Reflection Model

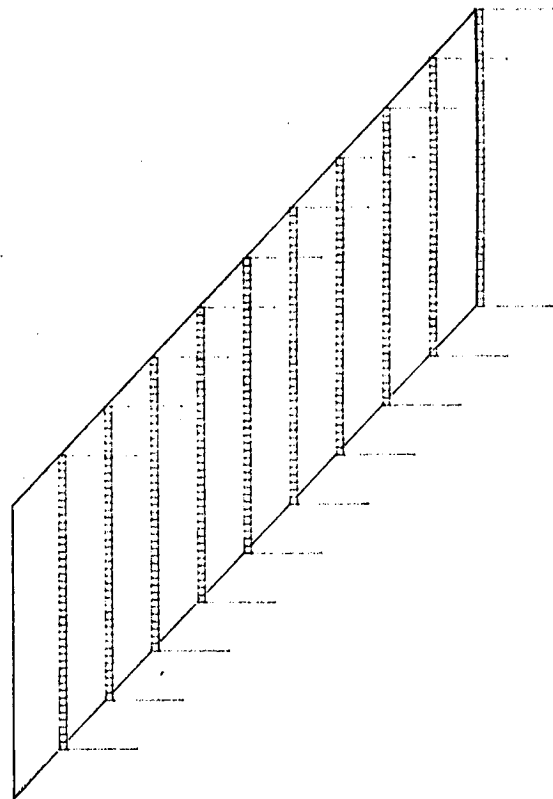


d) Gaussian Exponential Depletion Model

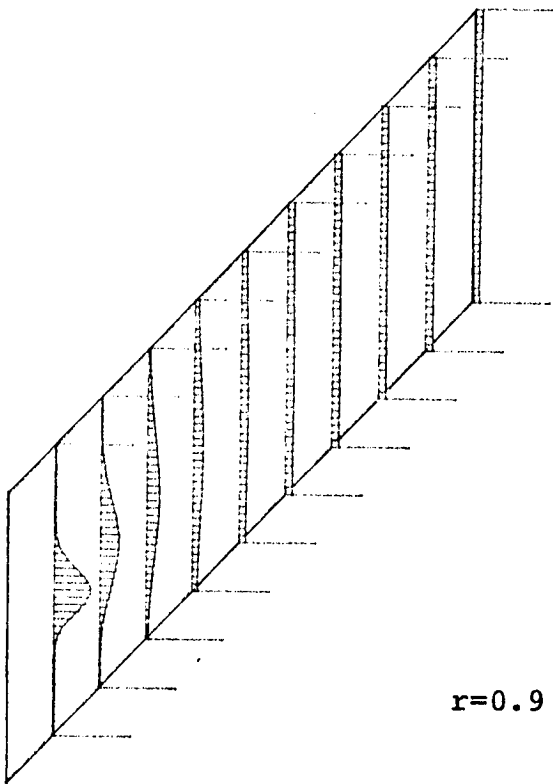
Figure 11. Predicted Crosswind Integrals for Neutral Atmosphere  
 $v_s = 0.2$  m/s



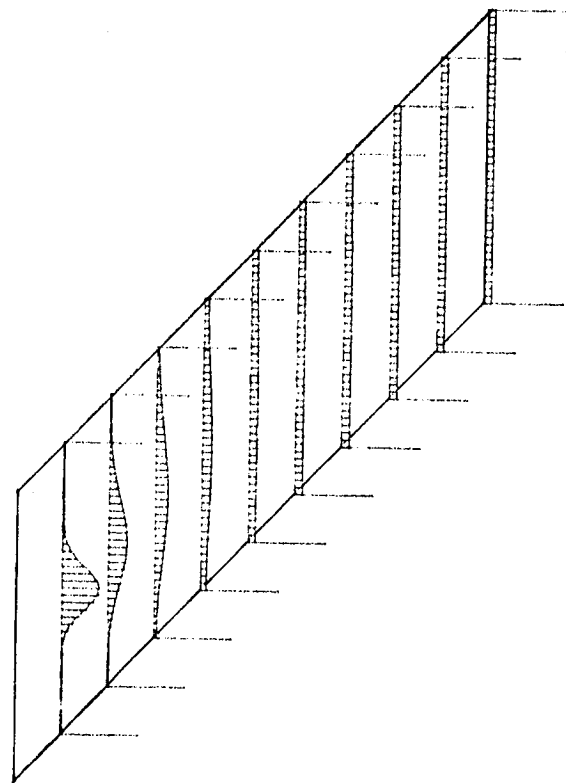
a) Diffusion Model



b) Perfect Vertical Mixing Model,  
Line Source



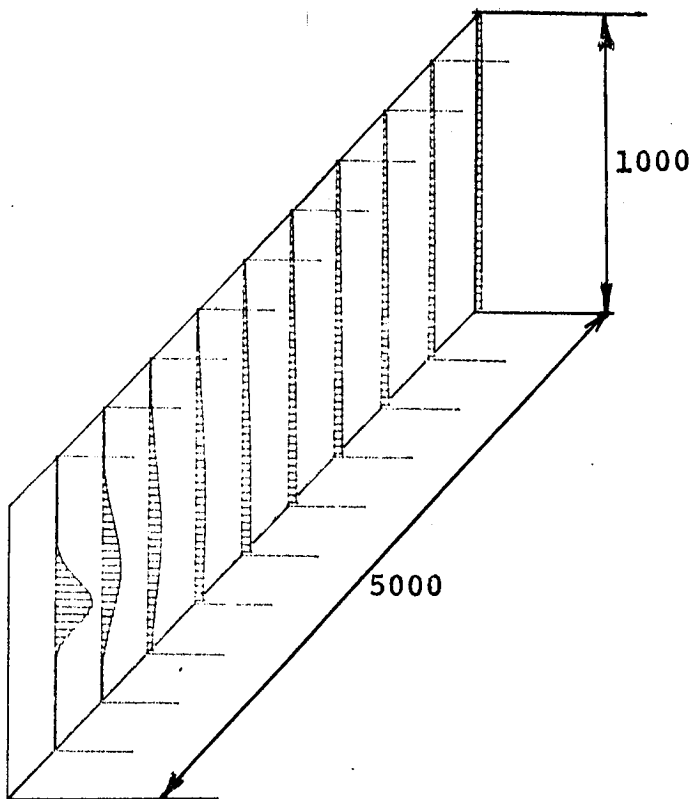
$r=0.9$



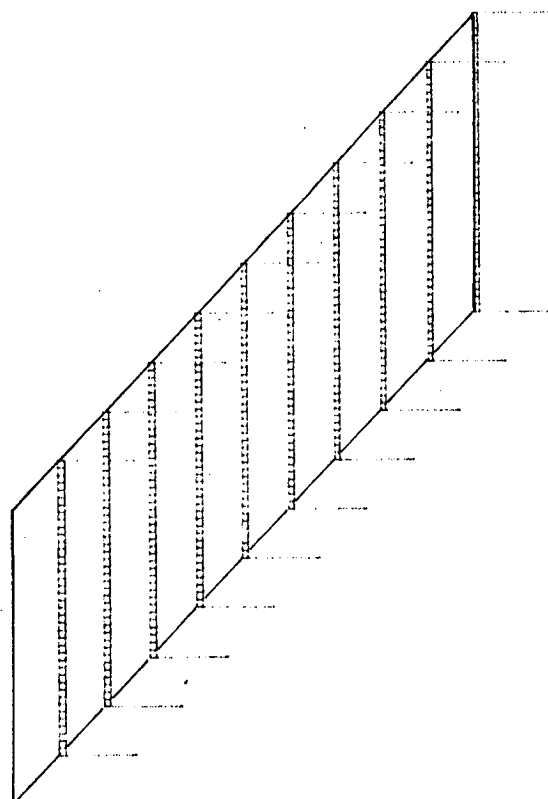
c) Gaussian Partial Reflection Model

d) Gaussian Exponential Depletion Model

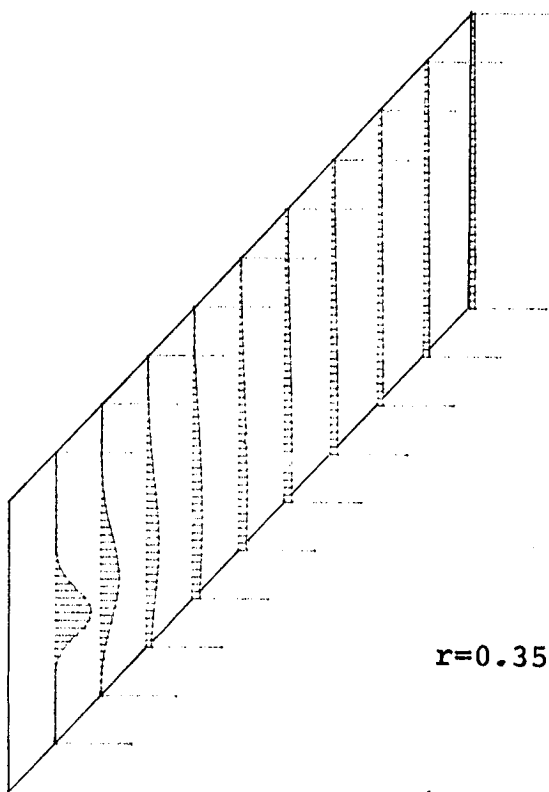
Figure 12. Predicted Crosswind Integrals for Unstable Atmospheres  
 $v_s = 0.02$  m/s



a) Diffusion Model

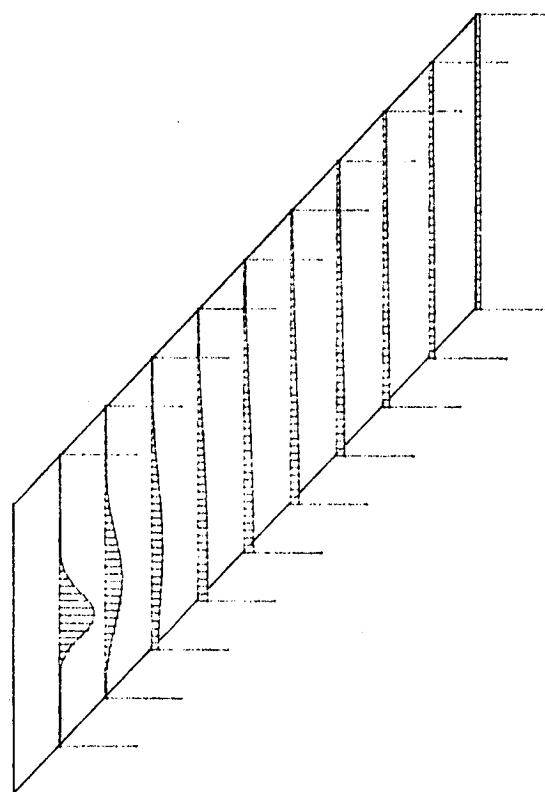


b) Perfect Vertical Mixing Model,  
Line Source



$r=0.35$

c) Gaussian Partial Reflection Model



d) Gaussian Exponential Depletion Model

Figure 13. Predicted Crosswind Integrals for Unstable Atmospheres  
 $v_s = 0.2$  m/s

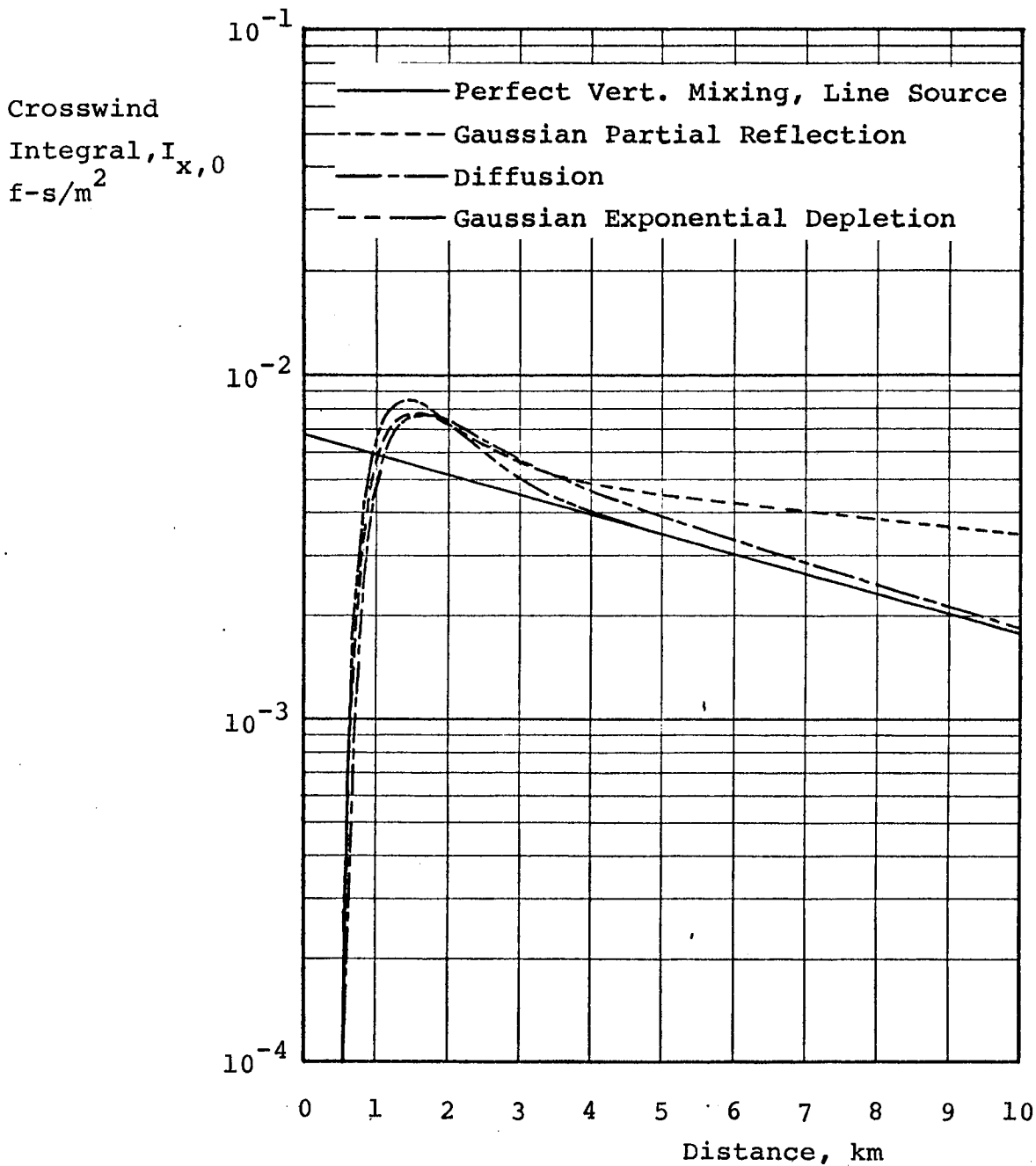


Figure 14. Variation of Crosswind Integral with  
Downwind Distance in Stable Atmosphere  
2 cm/s fall velocity

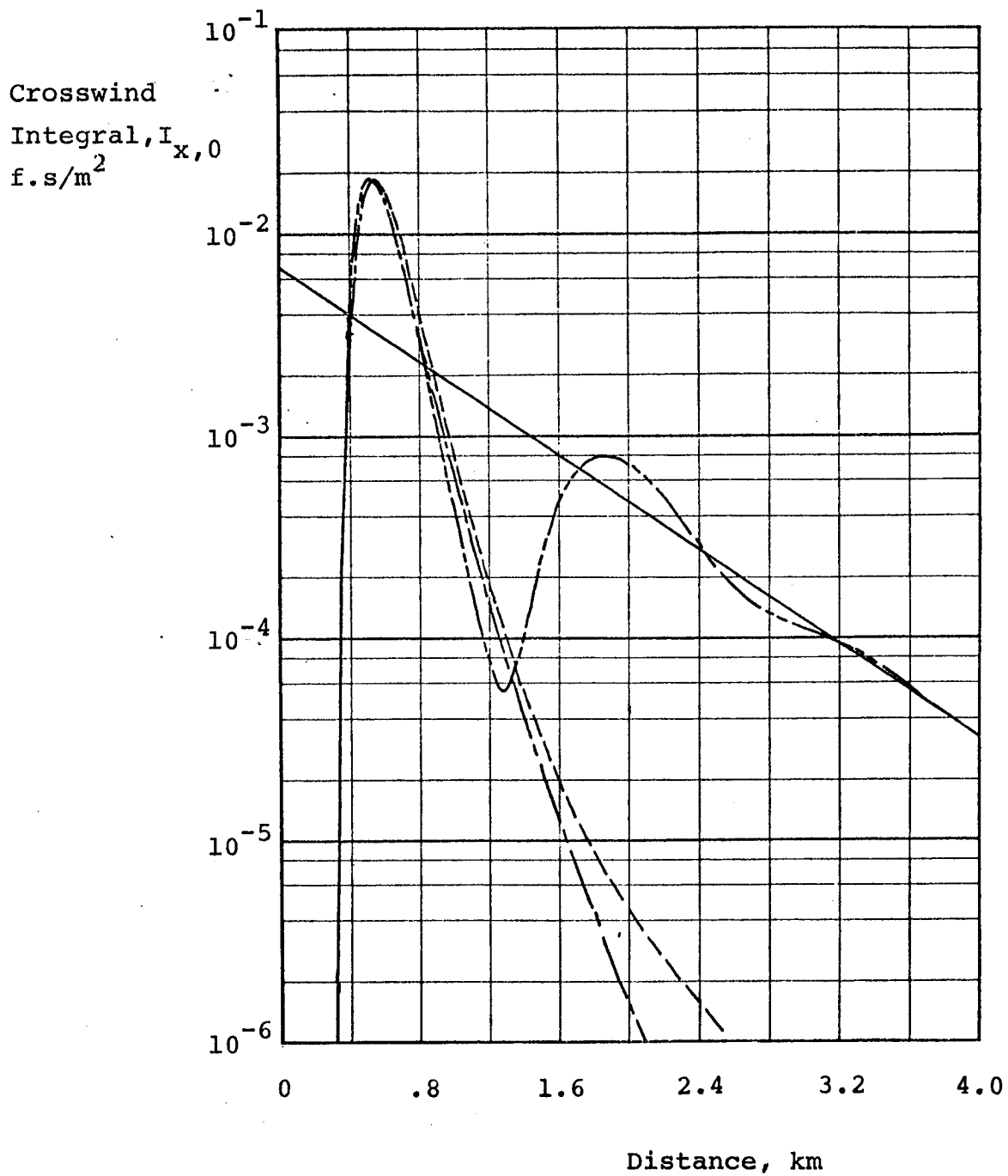


Figure 15. Variation of Crosswind Integral  
with Downwind Distance in Stable Atmosphere  
Fall Velocity 20 cm/s

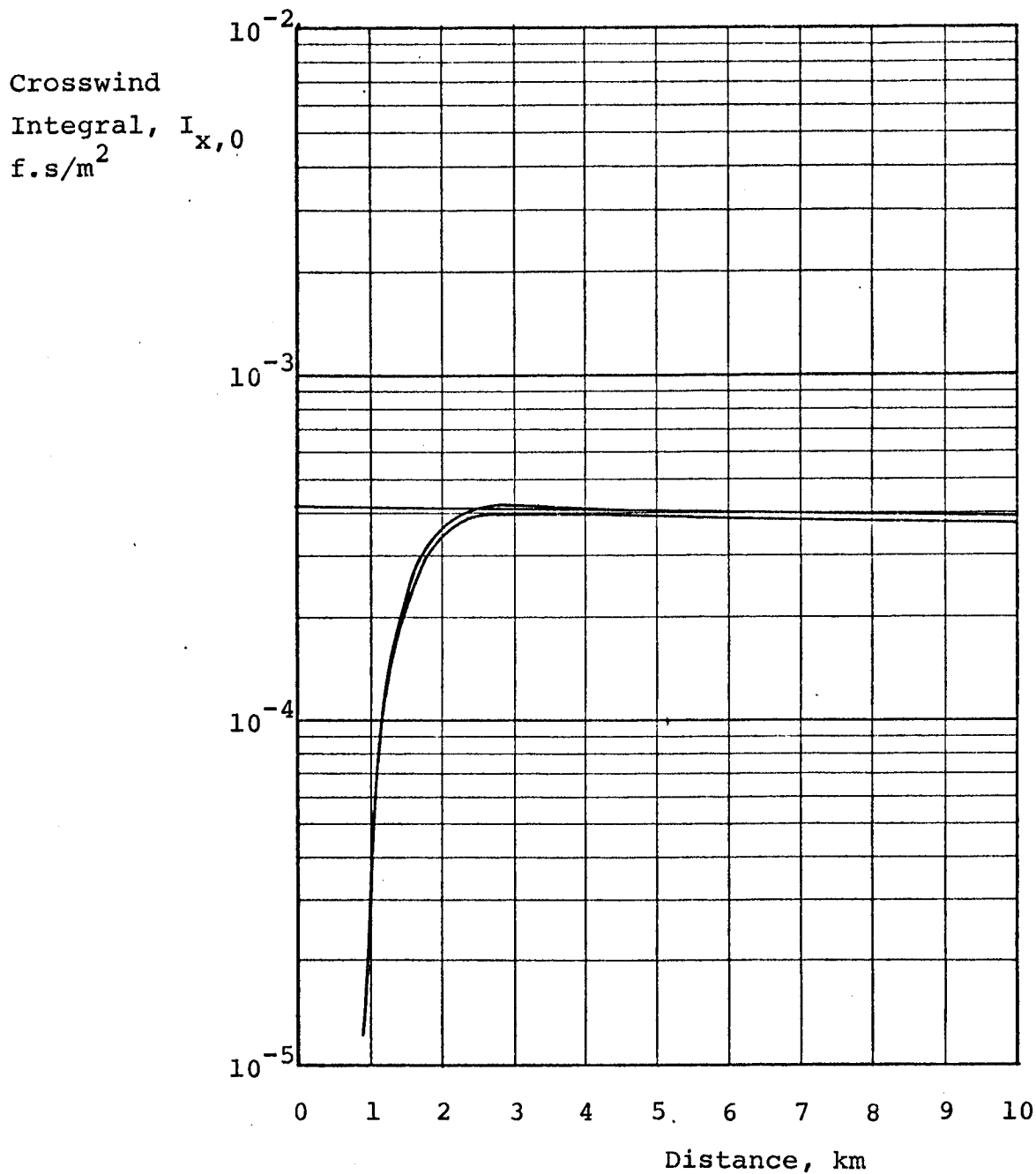


Figure 16. Variation of Crosswind Integral  
with Downwind Distance in Neutral Atmosphere  
Fall Velocity 2 cm/s



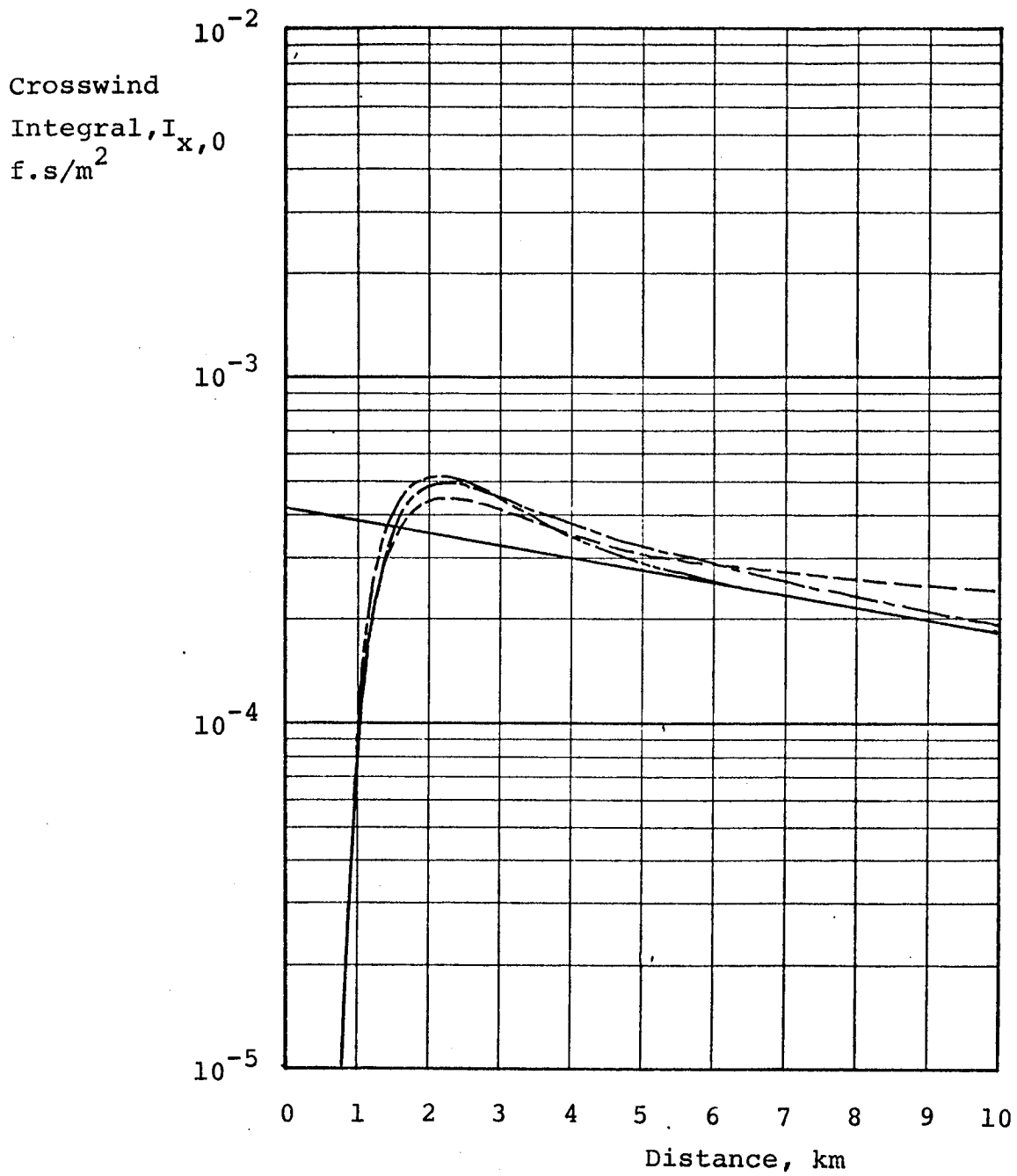


Figure 17. Variation of Crosswind Integral  
with Downwind Distance in Neutral Atmosphere  
Fall Velocity 20 cm/s

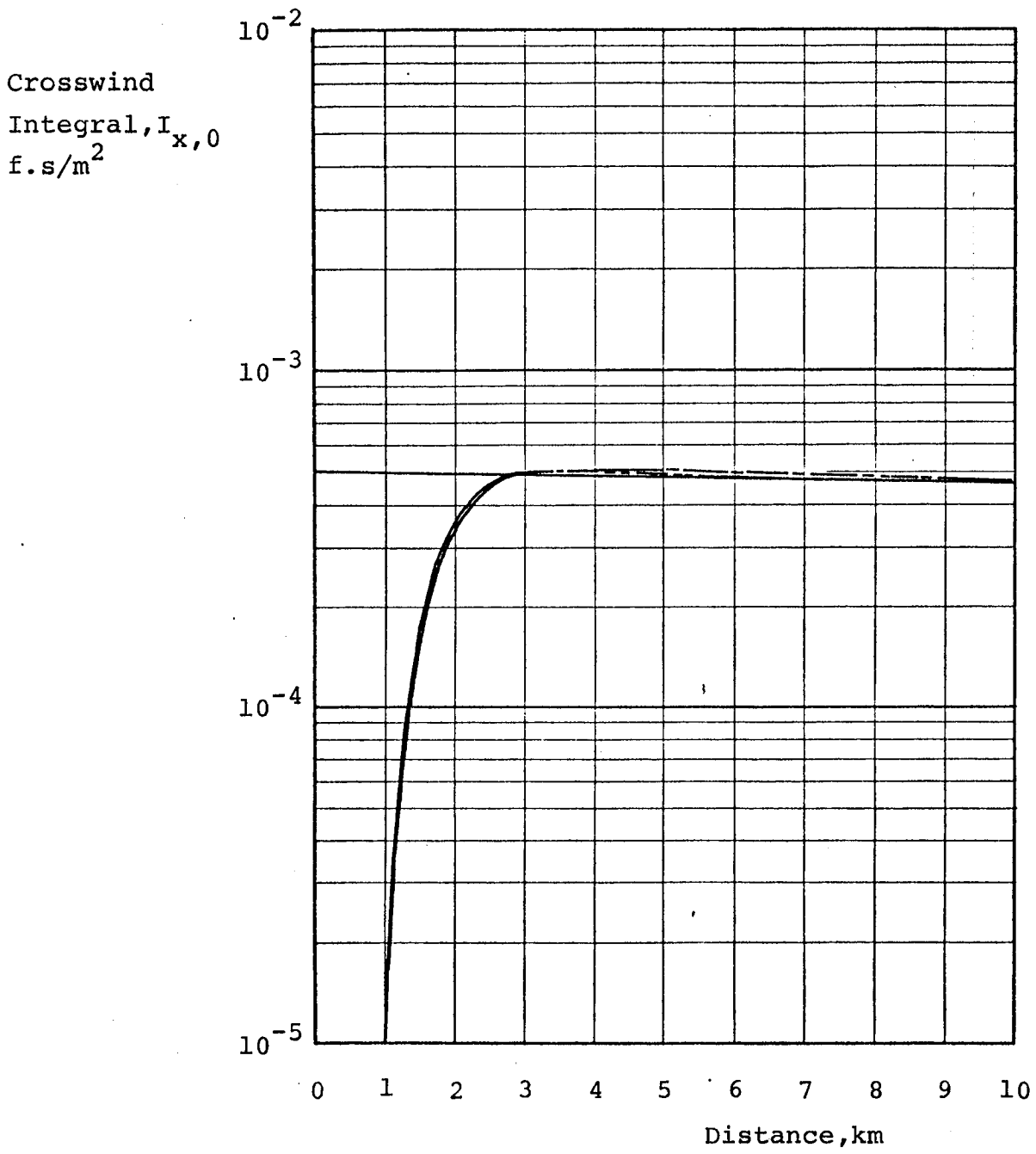


Figure 18. Variation of Crosswind Integral with Downwind Distance in Unstable Atmosphere, 2cm/s Fall Velocity.

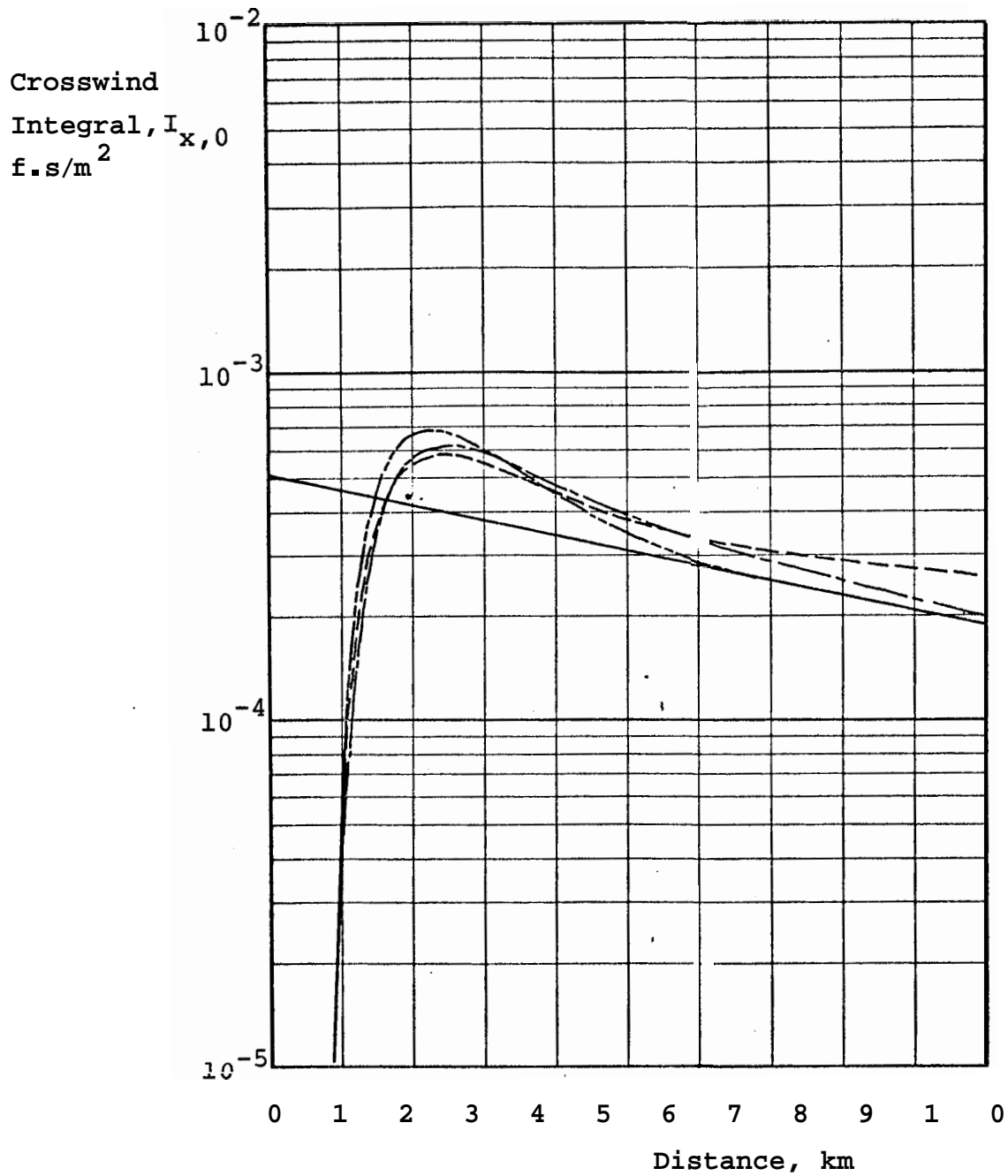


Figure 19. Variation of Crosswind Integral with Downwind Distance in Unstable Atmosphere 20 cm/s Fall Velocity.

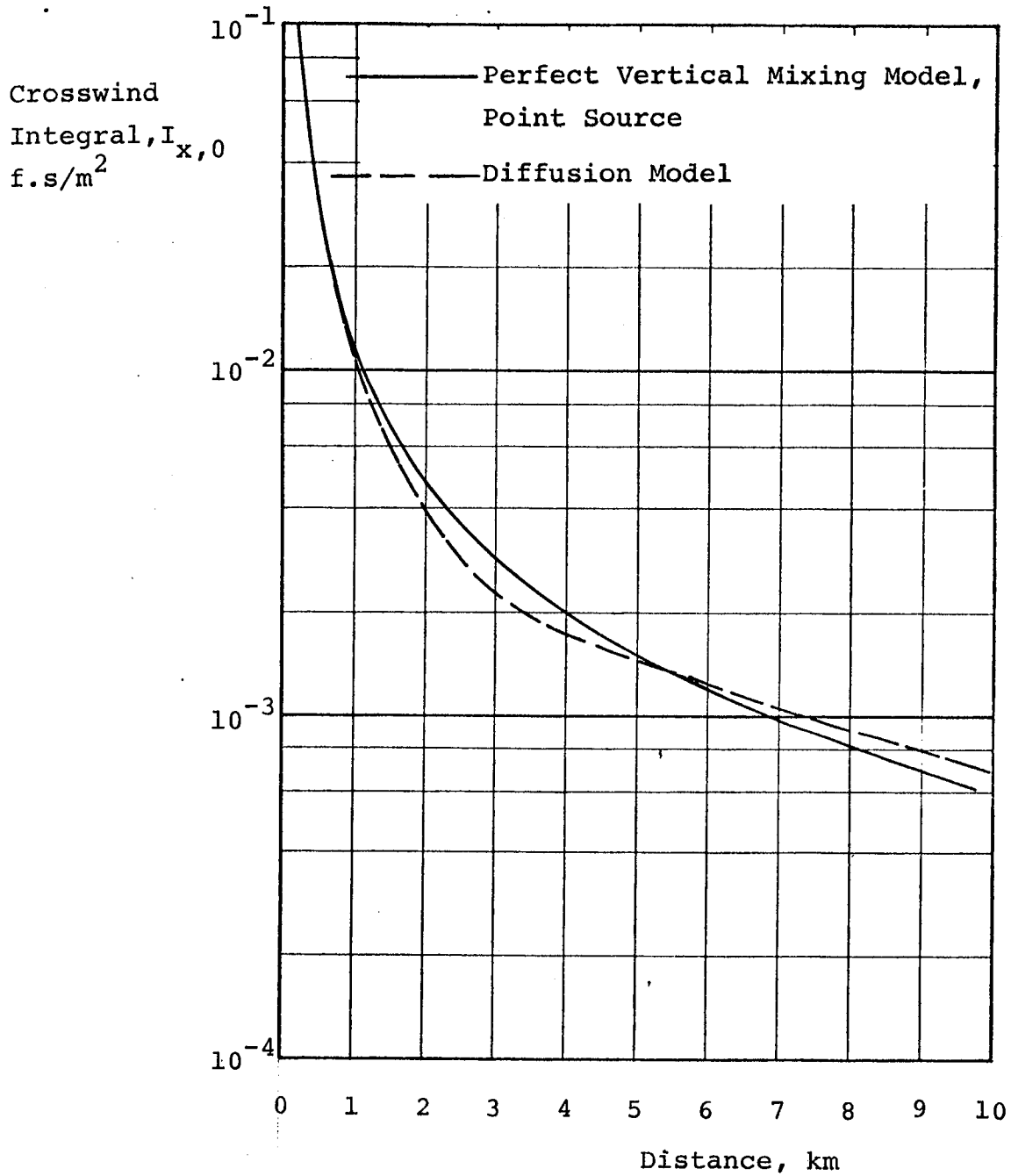


Figure 20. Unit Crosswind Integral for Ground-Based Point Source in Unstable Atmosphere and 2cm/s Fall Velocity.

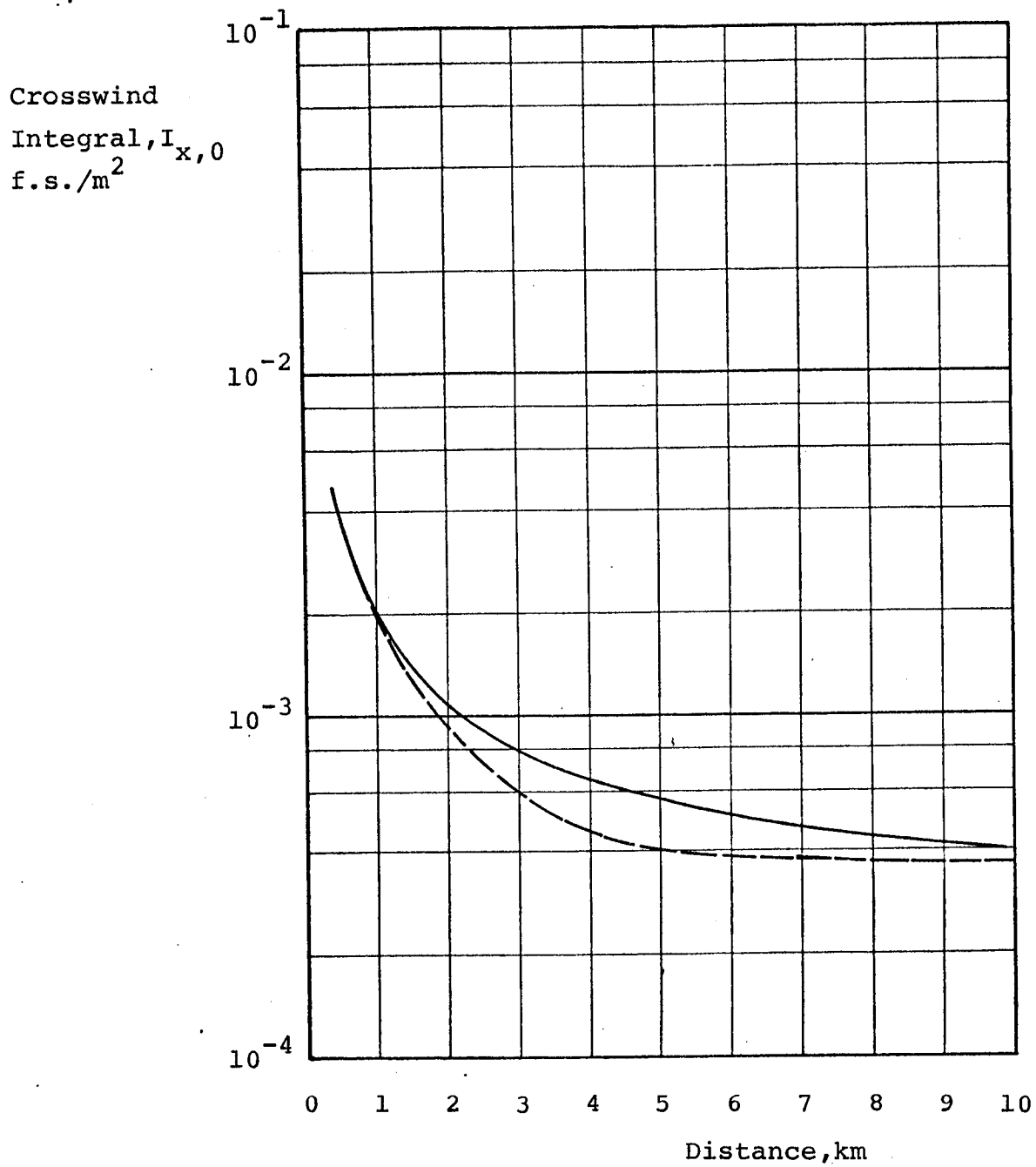


Figure 21. Unit Crosswind Integral for Ground-Based Point Source in Neutral Atmosphere and 2cm/s Fall Velocity.

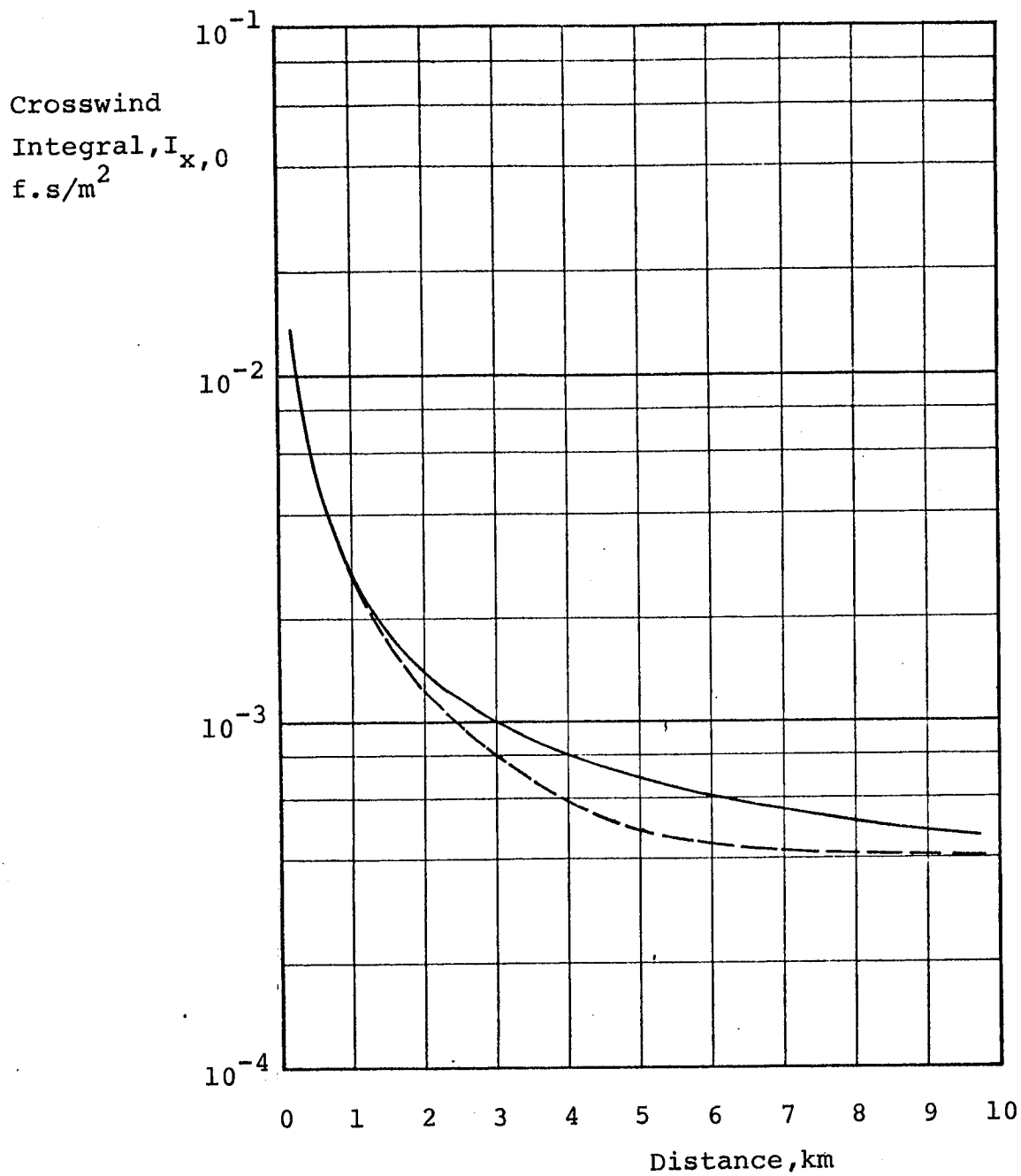


Figure 22. Unit Crosswind Integral for Ground-Based Point Source in Stable Atmosphere and 2cm/s Fall Velocity.

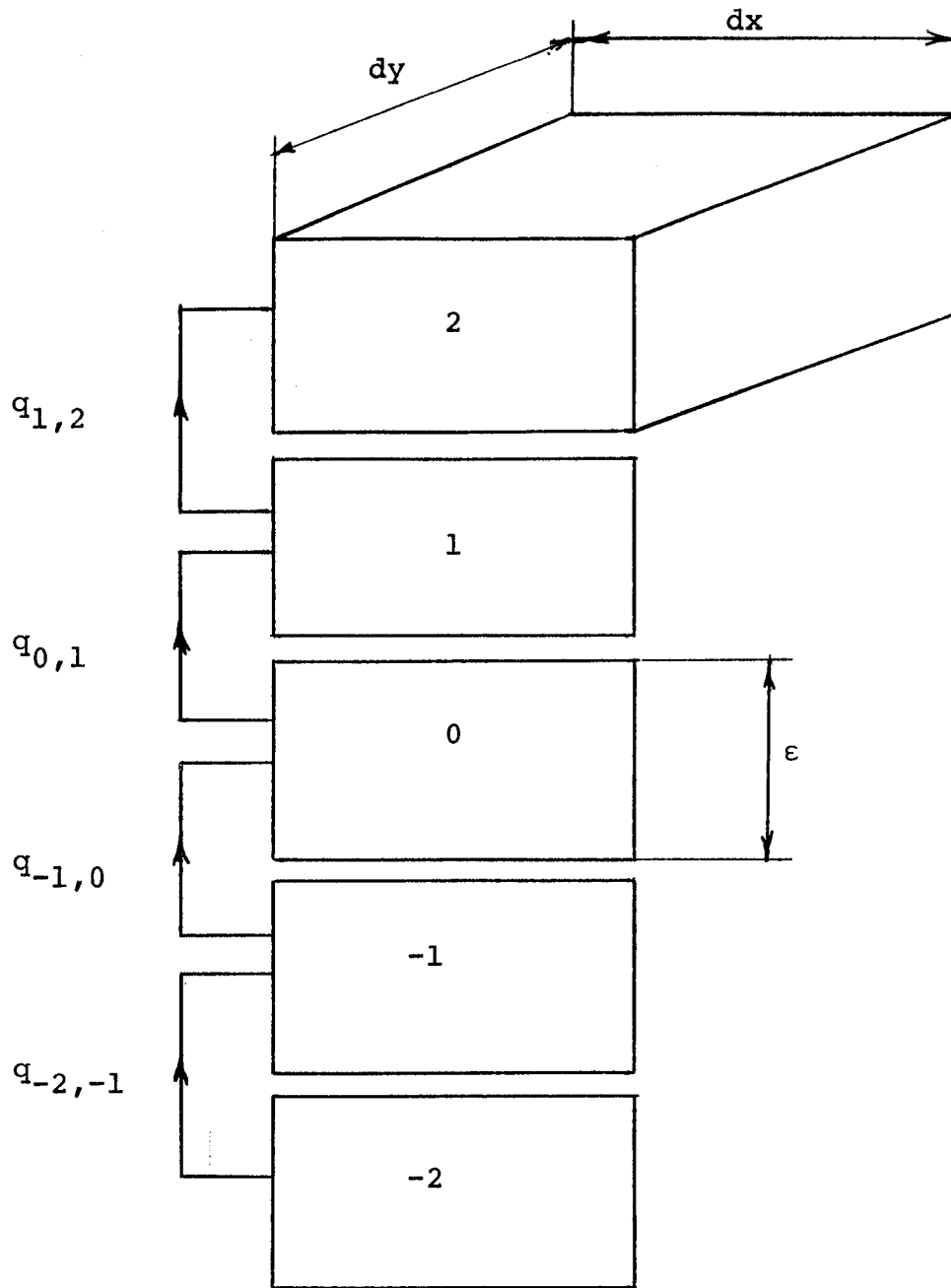


Figure 23. Finite Element Model for Atmospheric Diffusion





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| 16. Abstract<br><br><p>Dissemination prediction models have been reviewed to determine their applicability to a risk assessment for airborne carbon fibers. The review showed that the Gaussian prediction models using partial reflection at the ground agreed very closely with a more elaborate diffusion analysis developed for this study. For distances beyond 10,000 m the Gaussian models predicted a slower fall-off in exposure levels than the diffusion models. This resulting level of conservatism was preferred for the carbon fiber risk assessment. The results also showed that the perfect vertical-mixing models developed herein agreed very closely with the diffusion analysis for all except the most stable atmospheric conditions.</p> |  |  |   |   |                   |
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