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CONSTRUCTION OF A LAGRANGIAN SIMILARITY DISTRIBUTION FUNCTION FOR A NON-STATIONARY ATMOSPHERIC DIFFUSION PROCESS

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1. INTRODUCTION

The dispersion behavior of a non-stationary source in a turbulent shear flow has long been of interest because it represents an initial building block in understanding the most fundamental dilution process in the lower atmosphere. In this study we consider a classic problem in the diffusion theory: a passive, ground released, instantaneous point source. Consequently, based on the knowledge of this particular source, the concentration distribution from varied geometries and varied emission duration may be obtained by proper integration over space and time.

The significance of a turbulent diffusion process is to examine the ensemble probability distribution of a "tagged" fluid particle in a turbulent medium over space and time. This probability distribution function is usually dependent on a particle's travel time and flow properties.

By introducing the concept of a velocity autocorrelation function, G.I. Taylor (1921) derived a comprehensive expression for the standard deviation of a particle's spatial displacement. However, the basic assumption of Taylor's work was homogeneous turbulence. In atmospheric flow, especially at the ground level, the applicability of homogeneous turbulent diffusion theory ceases to be valid due to the characteristics of shear. Many efforts have been made to study diffusion behaviors in shear flows. The concept of eddy diffusivity (K-theory) has been widely accepted to close the turbulent transport equation. With a uniform velocity model, the K-equation can simply be transformed into a heat conduction equation. Unfortunately, uniform velocity models are far from adequate in describing the real transport process near the ground level. In addition, the uniform diffusivity assumption has been shown invalid in boundary layer flows (Hinze, 1959; Monin and Yaglom, 1971). However, a realistic model containing a non-uniform velocity profile and a non-uniform diffusivity distribution presents great analytic difficulties. The difficulties were often found in applying the information of diffusion studies to environmental sciences (Singer and Freudenthal, 1972).

In this study, we will use the Lagrangian Hypothesis incorporated with the governing transport equation containing a logarithmic velocity profile and linear diffusivity distribution. The previous analytic contributions due to Chatwin (1968) and Putta-Cermak (1971) in similar studies will also be described.

2. ANALYSIS

Based on conservation of mass, the transport equation in a fully developed turbulent boundary layer can be written as:

$$\frac{\partial c}{\partial t} + u(z)\frac{\partial c}{\partial x} = \frac{\partial}{\partial y}\left(K_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial c}{\partial z}\right) \qquad (1)$$

where

- c local mean concentration
- t time
- x longitudinal coordinate
- y lateral coordinate
- z vertical coordinate
- u mean velocity at x-direction
- K_y eddy diffusivity at y-direction
- K_z eddy diffusivity at z-direction

The longitudinal diffusion term $\frac{\partial}{\partial x} K_x \frac{\partial c}{\partial x}$ is neglected because it is, by order of magnitude, smaller than the mean convective term $u \frac{\partial c}{\partial x}$ (Monin and Yaglom, 1971). For a ground released instantaneous source, the initial condition reads:

I.C.: $c(x,y,z,t) = \delta(0,0,0,0)$

where δ is the Dirac-delta function. In a half-space with a reflecting floor, the boundary condition reads:

B.C.: $c, \frac{\partial c}{\partial x}, \frac{\partial c}{\partial y}, \frac{\partial c}{\partial z} \rightarrow 0$ at $x, y \rightarrow \pm\infty$
$z \rightarrow +\infty$

and $K_z \frac{\partial c}{\partial z} = 0$ at $z = 0$.

From Prandtl's mixing theory, the vertical momentum eddy diffusivity is a linear function of z. In a neutrally stratified turbulent flow, the Reynold's analogy simply states that the momentum and mass transfer mechanisms are essentially the same. Hence, one can define vertical mass eddy diffusivity as:

$$K_z = k u_* z$$

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where k is Karman's constant (=0.4 in air), u_* is the shear velocity. Since the transport process occurs mainly at the ground level, consequently the mean velocity profile can take a logarithmic form:

$$u(z) = \frac{u_*}{k} \ln\left(\frac{z}{z_0}\right) ,$$

where z_0 is the roughness parameter. The lateral eddy diffusivity can be assumed to be proportional to K_z[*], i.e., $K_y = A K_z = A k u_* z$, in which A is a constant. Thus, the complete transport equation reads:

$$\frac{\partial c}{\partial t} + \frac{u_*}{k} \ln\left(\frac{z}{z_0}\right) \cdot \frac{\partial c}{\partial x} = \frac{\partial}{\partial y}\left(A k u_* z \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(k u_* z \frac{\partial c}{\partial z}\right) . \tag{2}$$

As stated at the beginning of this paper, the complete solution for the transport equation with a nonlinear velocity profile and a non-uniform diffusivity distribution has not yet been obtained in any case. In this work, we apply the direct integration over the y and z axes to eliminate the sum of the orders of the differential equation. The lost information during the integrations will be evaluated by using the consequence of the Lagrangian Similarity Hypothesis.

First of all, when we apply integration to (2) over y direction, we obtain:

$$\frac{\partial L}{\partial t} + \frac{u_*}{k} \ln\left(\frac{z}{z_0}\right) \frac{\partial L}{\partial x} = \frac{\partial}{\partial z}\left(k u_* z \frac{\partial L}{\partial z}\right) \tag{3}$$

where

$$L(x, z, t) = \int_{-\infty}^{\infty} c(x, y, z, t)\, dy .$$

$L(x,z,t)$ is the marginal distribution of $c(x,y,z,t)$. It also has the significance of a concentration distribution from an instantaneous line source due to its independence of y.

If we again integrate (3) over x-domain, we obtain:

$$\frac{\partial L_*}{\partial t} = \frac{\partial}{\partial z}\left(k u_* z \frac{\partial L_*}{\partial z}\right) \tag{4}$$

where

$$L_*(z, t) = \int_{-\infty}^{\infty} L(x, z, t)\, dx .$$

$L_*(z,t)$ is thus the marginal distribution of $L(x,z,t)$. One can immediately solve (4) incorporated with the corresponding boundary conditions:

$$L_*(z, t) = \frac{1}{k u_* t}\, e^{-\frac{z}{k u_* t}} . \tag{5}$$

L_* can also be taken as the concentration distribution of an infinite plane (x-y) source at z=0. One can thus recognize that L_* has a form of a negative exponential distribution in z-space with a parameter of $\frac{1}{k u_* t}$. Consequently, L_* has a centroid at $k u_* t$ and a standard deviation of $k u_* t$.

[*] This may not be the best diffusivity model for K_y. However, after the integration over y and using a polynomial expansion in lateral direction, as we will show later, the functional form of K_y is not strictly important.

The centroid of a "puff" at any instant on the horizontal plane (x-y plane) can be evaluated by directly taking the first moment of equation (2). Because of the plane homogenity, the horizontal concentration distribution should be symmetric also w.r.t. y (this is true because the transport equation is linear; symmetry in momentum transport due to symmetric flow configuration may not always be true, for instance, the asymmetric vortex shedding behind a cylinder); i.e.,

$$\bar{y} = \int_{-\infty}^{\infty} y \cdot c(x, y, z, t)\, dy = 0 . \tag{6}$$

The trajectory of $\bar{x}$ is:

$$\bar{x} = \int_{-\infty}^{\infty} x \cdot c(x, y, z, t)\, dx = \frac{u_* t}{k}\left[\ln \frac{u_* t}{z_0 e^{\gamma}} - 1\right] . \tag{7}$$

The implicit trajectory of $\bar{z}$ can also be evaluated to be

$$\frac{\bar{z}}{z_0}\left[\ln \frac{\bar{z}}{z_0} - \gamma - 1\right] = \frac{k^2 \bar{x}}{z_0} . \tag{8}$$

Note that in the integration processes (3) and (4) we have reduced the sum of the orders of the governing equation to only a z-t dependent equation. However, it was done at the expense of losing the concentration distribution in y and x directions. In other words, we have obtained the exact expression for $L_*(z,t)$ where

$$L_*(z, t) = \int_{-\infty}^{\infty} L(x, z, t)\, dx = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c(x, y, z, t)\, dy\, dx .$$

In order to find a general expression of L and c, one can simply apply an infinite series expansion over x and y, namely

$$L(x, z, t) = L_*(z, t) \cdot X(x \mid z, t) \tag{9}$$

and

$$c(x, y, z, t) = L(x, z, t)\, Y(y \mid x, z, t) . \tag{10}$$

The selection of functional forms of conditional distribution functions X and Y will be discussed below.

3. SIMILARITY HYPOTHESIS AND SIMILARITY MOMENTS

The Lagrangian Similarity Hypothesis was first suggested by G.K. Batchelor (1959). The hypothesis states:

"At the ground level, the statistical properties of the velocity of a marked fluid particle, at time t after release from the ground, are functions of shear velocity u_* and travel time t."

The validity of this hypothesis and its application to turbulent diffusion were confirmed by Gifford (1962) and Cermak (1963). The similarity parameters from the definition are:

$$\beta = \frac{x - \bar{x}}{a u_* t} , \quad \zeta = \frac{y}{g u_* t} , \quad \text{and} \quad \eta = \frac{z}{b u_* t} . \tag{11}$$

The most important consequence from the hypothesis is that the standard derivations of the concentration distribution at time t are linearly proportional to $u_* t$, i.e.,

$$\sigma_x = a u_* t \,, \quad \sigma_y = g u_* t \quad \text{and} \quad \sigma_z = b u_* t \,. \tag{12}$$

These can be shown on the ground of dimensional analysis (Chatwin, 1968). From (5), the form of negative exponential distribution gives immediately the value of σ_z as $k u_* t$. Thus, vertical diffusion constant b is equivalent to Karman's constant 0.4.

Note that Chatwin (1968) was the first to analyze a transport equation with logarithmic velocity profile and linear vertical diffusivity. In order to simplify the problem, he only discussed a two-dimensional case. The equivalent situation is to start the problem from (3) instead of (2). He also found that the transformed transport equation in the $\beta - \eta$ space is

$$\frac{\partial^2 L_s}{\partial \eta^2} + (\eta + 1)\frac{\partial L_s}{\partial \eta}\left(\beta - \frac{1}{ak} \ln \eta e^{\gamma}\right)\frac{\partial L_s}{\partial \beta} + 2L_s = 0$$

in which γ is Euler's constant (0.577)

$$\text{and } L_s(\beta, \eta)^{\dagger} = a k u_*^2 t^2 L(x, z, t) \,. \tag{13}$$

This equation is apparently too complicated to be solved. Chatwin applied the Aris Moment method (Aris, 1956), and obtained a series of ordinary differential equations:

$$\eta \frac{d^2 B_k}{d\eta^2} + (\eta + 1)\frac{dB_k}{d\eta} - (\eta - 1) B_k = \frac{k B_{k-1}}{ak} \ln \eta e^{\gamma} \,, \quad k = 0, 1, 2, \ldots \tag{14}$$

where

$$B_k(\eta) = \int_{-\infty}^{\infty} \beta^k L_s(\beta, \eta)\, d\beta \,.$$

The first two equations were solved by Chatwin (1968):

$$B_0(\eta) = e^{-\eta}$$

$$B_1(\eta) = \frac{e^{-\eta}}{ak}(\ln \eta + \gamma - 1) + \frac{\int_\eta^\infty \frac{e^{-\eta}}{\eta}\, d\eta}{ak} \,.$$

Putta and Cermak (1971) continued the calculation and obtained a complicated analytic expression for B_2 by using the following identity:

$$\lim_{\eta \to 0} \int_\eta^\infty \frac{e^{-\eta}}{\eta}\, d\eta + e^{-\eta} \ln(\eta e^{\gamma}) \longrightarrow 0$$

so

$$\begin{aligned} B_2(\eta) = \frac{1}{a^2 k^2}\Bigg[& 2\int_\eta^\infty \frac{e^{-\eta}}{\eta}\, d\eta \ln(\eta e^{\gamma}) + \ln^2(\eta e^{\gamma}) e^{-\eta}(\eta + 2) \\ & - 2\eta \int_\eta^\infty \frac{e^{-\eta}}{\eta}\, d\eta + 3e^{-\eta} - (\eta + 1)\big(\Gamma''(1, \eta) \\ & + 2\gamma \Gamma'(1, \eta) + \gamma^2 e^{-\eta}\big)\Bigg] \end{aligned} \tag{15}$$

where

$$\Gamma^{(i)}(j, \eta)$$

is i^{th} derivative of incomplete gamma function with respect to parameter j.

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† The subscript s in this paper indicates the function is in the similarity space.

The most important result of this work was the obtaining of the longitudinal diffusion constant a after a series of analytic integrations. The a-value was predicted to be:

$$a = 1.5 \,.$$

Note that a-value has been studied by various authors (Cermak, 1963) and suggested to be within 1.0 to 4.0.

Another important contribution from Putta's and Cermak's work was to show that the longitudinal standard derivation is insensitive to the height. The normalized third moment, or the skewness, was estimated to be -1.

4. CONSTRUCTION OF A COMPLETE DISTRIBUTION FUNCTION

The present authors continued and extended the study from a line source to a point source. In addition, the authors have conducted a wind tunnel study of this problem. The experiment was carried out in a micrometeorological wind tunnel at Colorado State University. An aerosol-filled gas bubble was released in a column of water to subsequently rise and burst at the floor of the wind tunnel (Yang and Meroney, 1972). Time-dependent concentrations at a fixed point were monitored with a laser light scattering measuring device. Figure 1 shows the experimental results of σ_x. One can see the longitudinal growth of a puff, although scattered, follows the trend of a = 1.5. The longitudinal skewness was also plotted in Figure 2. Note that most of the skewness was slightly less than the predicted value of -1.0 (absolute values). This is due to the finite instrumentational resolution. In addition, any long-trailed distribution function has greater contribution to the 3rd moment than to the 2nd moment from the tail.

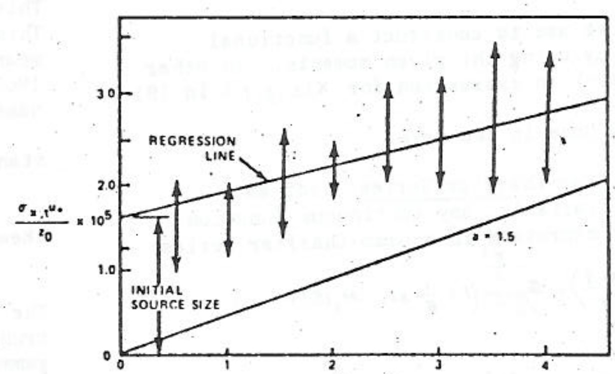

Figure 1 LONGITUDINAL STANDARD DEVIATION PLOT (WIND TUNNEL DATA)

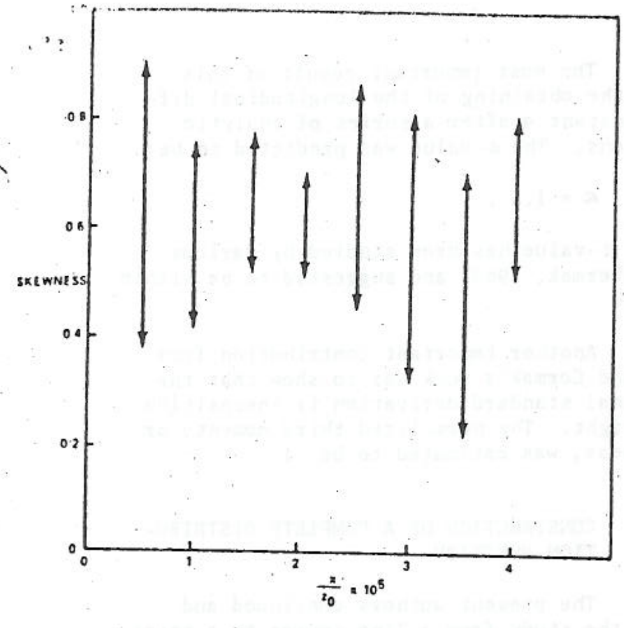

Figure 2 LONGITUDINAL SKEWNESS PLOT (WIND TUNNEL DATA)

Authors also examined a recent field study of the similar problem. Full scale concentration measurements were conducted by Pacific Northwestern Laboratory at Hanford Reservation, Washington (Nickola, 1971). The a-value was found to be between 1.3 and 1.7. (See Yang and Meroney, 1972.)

4.1 LONGITUDINAL DISTRIBUTION FUNCTION

From equation (14) the three analytic moments in the longitudinal coordinate are obtained, i.e.,

$$\bar{x} = \frac{u_* t}{k}\left(\ln \frac{u_* t}{z_0 e^{\gamma}} - 1\right),$$

$$\sigma_x = 1.5\, u_* t$$

and skewness = -1.

We are to construct a functional expression by using the given moments. In other words, we seek an expression for $X(x|z,t)$ in (9).

This can be done in two ways:

Gram-Charlier Series. For an independent variable, any continuous function h(s) can be expressed in a Gram-Charlier Series:

$$f(S) = f\left(\frac{s-\bar{s}}{\sigma}\right) = \frac{e^{-\frac{S^2}{2}}}{\sqrt{2\pi}}\left(1 + \frac{1}{6}\, sk. \cdot H_3(S) + \ldots\right) \quad (17)$$

where

S $= \frac{s-\bar{s}}{\sigma}$ is a normalized parameter,

$\bar{s}$ = mean of the original distribution function,

σ = standard derivation of the original distribution function.

$H_3(S)$ = S^3-$3S^3$ Hermite polynomials of degree 3,

and

sk. = skewness of the original distribution $= \frac{\int_s (s-\bar{s})^3 h(s)\, ds}{\sigma^{3/2}}$.

This series expression states that any distribution function in the normalized space S can be taken as a perturbed form of a standard normal $\frac{1}{\sqrt{2\pi}} e^{-S^2/2}$ (Kendall and Sturt, 1963). The improvement of fitness by taking higher than 3rd moments in the Gram-Charlier series was given by Cramer (1957). The attractive feature of this series is that it takes normalized moments as independent coefficients. Since the similarity parameters are already normalized by definition, the truncated expression for $X_s(\beta)$ thus reads:

$$X_s(\beta) = \frac{e^{-\frac{\beta^2}{2}}}{\sqrt{2\pi}}\left[1 - \frac{1}{6}(\beta^3 - 3\beta)\right]. \quad (18)$$

Inverse-gamma distribution. The Gram-Charlier series is a general form of a distribution function which applies given normalized moments to construct a truncated series. However, in many cases, a set of given moments can also be used to select a standard distribution function. There are several advantages to the use of a standard distribution function. First, one can develop a better functional feeling since the trends of most standard distribution functions can be found (Parzen, 1967). Second, the intermittent "negative concentration" in a truncated series can be avoided. Third, most standard distributions have a relatively simpler functional form than the Gram-Charlier series. For instance, the chosen gamma distribution because of its one-way skewness in this study has a negative exponent of the first order. In the Gram-Charlier series, there is always a second degree term in the exponent.

Examining the general shape of a gamma distribution in space ω one has to apply the following transformation

$$\omega' = \text{constant} - \omega$$

in order to fit the longitudinal distribution. This is actually an inverse gamma distribution. This is a 2-parameter family with a "floating mean". Based on the given knowledge, (Parzen, 1967), we have the following set of conditions, namely,

standard deviation: $\sigma_\beta = \frac{\sqrt{r}}{\lambda} = 1$ and

skewness: $sk_\beta = -\frac{2}{r^{1/2}} = -1$.

The result reads: $\lambda = 2.0$ and $r = 4.0$. The truncated Gram-Charlier series and the inverse gamma distribution were plotted in Figure 3. One can see there is not significant difference between two distribution functions.

Note that one cannot justify which distribution, the Gram-Charlier series or inverse gamma, is a better description of the exact cloud concentration distribution, unless higher moments are obtained.

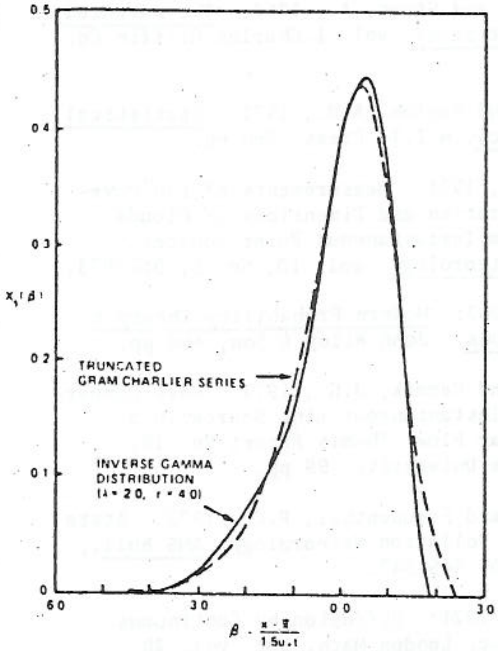

Figure 3 LONGITUDINAL SIMILARITY DISTRIBUTION: TRUNCATED GRAM-CHARLIER SERIES REPRESENTATION AND INVERSE-GAMMA DISTRIBUTION REPRESENTATION

To obtain the 4th moment in equation (14) one would, however, face tremendous analytic complexities. This effort may not be so rewarding in gaining further knowledge of the distribution shape. (Cramer, 1957). Hence, we propose to use the inverse-gamma distribution to close the solution. By "closed form", we mean that the integrated value is exactly unity as a distribution function is normally defined.

Using the chosen values ($\lambda = 2$, $r = 4$), one can write the similarity profile as:

$$X_s(\beta) = \frac{2}{\Gamma(4)}\left[2\cdot(2-\beta)\right]^3 e^{-2(2-\beta)} \qquad \beta = -\infty, 2$$

where

$$\Gamma(4) = 3\cdot 2\cdot 1 = 6\ ;$$

therefore,

$$X_s(\beta) = \frac{8}{3}(2-\beta)^3 e^{-2(2-\beta)} \qquad \beta = -\infty, 2 .$$

The explicit form is

$$X(x|t,z) = \frac{8}{3au_* t}\left[2 - \frac{x-\bar{x}}{au_* t}\right]^3 e^{-2\left[2-\frac{x-\bar{x}}{au_* t}\right]} \qquad (19)$$

where

$$\bar{x} = \frac{u_* t}{\kappa}\left[\ln\frac{k u_* t}{z_0 e^{r}} - 1\right] .$$

The line source distribution in the β-η domain thus reads:

$$L_s(\beta,\eta) = \frac{8}{3}(2-\beta)^3 e^{-2(2-\beta)}\, e^{-\eta} . \qquad (20)$$

4.2 COMPLETE DISTRIBUTION FOR AN INSTANTANEOUS POINT SOURCE

To extend a line source solution to a point source, one can simply expand the Gram-Charlier series in the lateral direction, i.e.,

$$c(x,y,z,t) = L(x,z,t)\,Y(y|x,z,t)$$

$$= L(x,z,t)\frac{e^{-\frac{\zeta^2}{2}}}{\sqrt{2\pi}\,g u_* t}\left[1+\frac{1}{6}\ (\text{skewness in } \zeta\text{-direction})\cdot(\zeta^3 - 3\zeta) + \dots\right] .$$

The 1st moment vanishes because

$$\int_{-\infty}^{\infty} c(x,y,z,t)\,y\,dy = \int_{-\infty}^{\infty} c_s(x,y,z,t)\frac{y}{g u_* t}\,d\frac{y}{g u_* t} = 0 .$$

From the same reason of symmetry, the skewness in ζ - direction vanishes;

$$\text{skewness in } \zeta\text{-direction} = 0 .$$

Therefore, one obtains

$$c(x,y,z,t) = L(x,z,t)\frac{e^{-\frac{\zeta^2}{2}}}{\sqrt{2\pi}\,g u_* t} \qquad (21)$$

Based on the experimental results (Fig. 4), the authors suggested

$$g = 1.0 . \qquad (22)$$

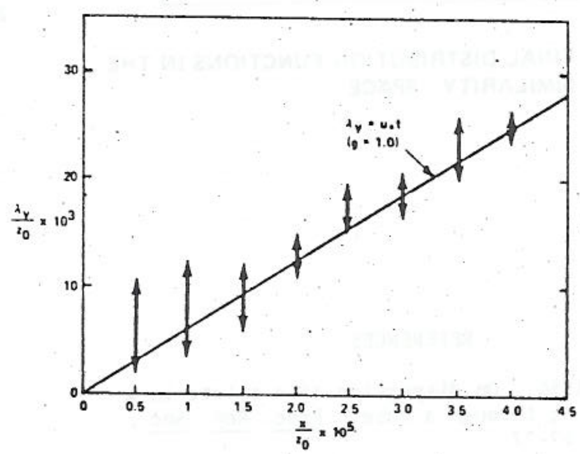

Figure 4 GROWTH OF HALF WIDTH OF CONCENTRATION IN THE LATERAL DIRECTION

Note that in Figure 4, the half widths (from center line to the one half of the maximum concentration) were plotted. This is because the data are presented in discrete points. In addition, for a normal distribution, the half width is proportional to standard deviation.

From equations (21), (22), (9), (19) and (5), the resulting closed form concentration distribution function for a passive, ground released, instantaneous point source reads:

$$c(x,y,z,t) = \frac{1.7331}{u_*^3 t^3}\, e^{-\left(4-2\beta+\frac{\zeta^2}{2}+\eta\right)}\cdot(2-\beta)^3 \qquad (23)$$

in which β, ζ and η were previously defined.

In similarity space, the distribution function has the following form:

$$c_s(\beta,\zeta,\eta) = \frac{8}{3}\, e^{-(4-2\beta)} \cdot (2-\beta)^3 \cdot \frac{e^{-\frac{\zeta^2}{2}}}{\sqrt{2\pi}} \cdot e^{-\eta} \quad . \quad (24)$$

Thus, this distribution function is actually composed of three distribution functions: an inverse-gamma distribution in β-domain, a normal distribution in ζ domain, and a negative distribution in η domain. These are illustrated in Figure 5.

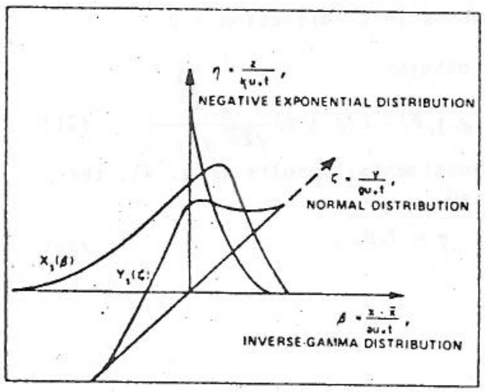

Figure 5 FINAL DISTRIBUTION FUNCTIONS IN THE SIMILARITY - SPACE

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