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DERIVATION OF HYPERBOLIC TURBULENT DIFFUSION EQUATION

By

Ronald E. Meyers

MAY 1967

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UNITED STATES ARMY ELECTRONICS COMMAND
ATMOSPHERIC SCIENCES LABORATORY, RESEARCH DIVISION
FORT HUACHUCA, ARIZONA

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Technical Report ECOM-6026

DERIVATION
of an
ATMOSPHERIC HYPERBOLIC TURBULENT
DIFFUSION EQUATION
(Preliminary Report)

By
Ronald E. Meyers

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ABSTRACT

A three dimensional hyperbolic differential equation based on finite correlated particle velocities is derived which is appropriate to modeling anisotropic turbulent diffusion in the atmosphere. Cauchy initial data, the mean wind, the Reynolds stress tensor, and a typical frequency of pulsation are required for complete solution. The outlines of plumes and puffs may be obtained with only knowledge of the Reynolds stress tensor and mean wind velocity. The classical parabolic diffusion equations are a limiting form of this hyperbolic model.

FOREWORD

This report is intended as a summary of preliminary efforts to derive a general diffusion equation more appropriate to atmospheric diffusion modeling than existing models.

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I. INTRODUCTION TO ATMOSPHERIC TURBULENT DIFFUSION

This phase space derivation of a hyperbolic turbulent diffusion equation is motivated by several less general random walk and hyperbolic diffusion models [6, 8, 13, 15, 16, 18, 19, 26] which appear to more reasonably represent the physical processes involved in atmospheric diffusion than any of the classical models. The basis for the classical models of turbulent diffusion, almost without exception, is one form or another of the parabolic diffusion equation. Even the semi-empirical Gaussian plume equation, the foundation for much recent diffusion studies, may be derived from a parabolic diffusion equation [3]. Recent reviews of the state of diffusion modeling in the lower atmosphere express a dissatisfaction with the degree of generality to which existing models may be extended, and agree that no comprehensive mechanism of turbulent diffusion has been modeled [3, 4, 5, 14]. It is significant that most recent reviews concerned with diffusion application omit serious consideration of hyperbolic systems such as those of Monin [19] and Goldstein [13] which are expressions of particle motions correlated as in the case of atmospheric turbulence. While these first efforts are not very general, they do provide certain features which allow a more realistic modeling compatible with practical applications. In the present hyperbolic model, the primary assumption, that diffusion can be represented by a Markov process in phase space, is suggested as being a less restrictive assumption than the corresponding assumption used in the derivation of the classical parabolic diffusion equation. The classical parabolic diffusion equation can be derived by assuming a Markov process in configuration space [1, 8, 10, 17]. Furthermore the classical assumption that the velocity necessary for the formulation of a continuity equation can be derived from the particle density gradient presents the paradoxical result that densities exist everywhere even a short time after a release. Thus particle paths exist for which there are no corresponding velocities. In the

phase space model the particles have velocities - finite velocities. The possibility exists then to relate the velocities of the diffusing particles to the velocities of the turbulent atmospheric fluid.

II. THEORETICAL DERIVATION OF TURBULENT DIFFUSION EQUATION

The derivation is based on two premises. The first is that turbulent diffusion can be described by statistical methods relating particle statistics to the statistics of the atmospheric turbulence field. The second is that the mean wind profile can be introduced into the turbulence field.

The turbulence field representation will be based on the "phase space" description of the probability density for a particle. We assume that the diffusion can be represented by a Markov process in phase space. The phase space representation of a particle has been investigated by Chandrasekhar [1], Kramers [17], Obukhov [22], Tchen [29], and Davies [8]. We shall start similarly to Chandrasekhar. In the Markov process in phase space, the probability density at $t+\Delta t$, $W(t+\Delta t)$, is derived from the probability density at t , $W(t)$.

$$W(\vec{r}, \vec{u}; t+\Delta t) = \iint W(\vec{r}-\Delta\vec{r}, \vec{u}-\Delta\vec{u}, t) \phi(\vec{r}-\Delta\vec{r}, \vec{u}-\Delta\vec{u}, \Delta\vec{r}, \Delta\vec{u}) d(\Delta\vec{u}) d(\Delta\vec{r}) \quad (1)$$

ϕ is the transition probability density in phase space, \vec{r} is the vector representation of the configuration space, and \vec{u} is the vector representation of the velocity space.

We now relate the increments of time and configuration space by

$$\Delta\vec{r} = \vec{u}\Delta t. \quad (2)$$

The transition probability density in phase space can now be represented by the transition probability density in velocity space and the Dirac delta function.

$$\phi = \phi(\vec{r}-\Delta\vec{r}, \vec{u}-\Delta\vec{u}, \Delta\vec{u}) \delta(\Delta\vec{r}-\vec{u}\Delta t) \quad (3)$$

The integration over the configuration space increment is now easily performed.

$$W(\vec{r}+\vec{u}\Delta t, \vec{u}, t+\Delta t) = \int W(\vec{r}, \vec{u}-\Delta\vec{u}, t) \phi(\vec{r}, \vec{u}-\Delta\vec{u}, \Delta\vec{u}) d(\Delta\vec{u}) \quad (4)$$

Both sides are expanded in a Taylor series about the point (\vec{r}, \vec{u}, t) .

$$W + W_t \Delta t + (\vec{u} \cdot \vec{\nabla} W) \Delta t + O(\Delta t^2) =$$

$$\int_{-\infty}^{+\infty} \left\{ W - \sum_i \frac{\partial W}{\partial u_i} \Delta u_i + \frac{1}{2} \sum_i \frac{\partial^2 W}{\partial u_i^2} (\Delta u_i)^2 + \sum_{i < j} \frac{\partial^2 W}{\partial u_i \partial u_j} \Delta u_i \Delta u_j + \dots \right\} \cdot$$

$$\left(\psi - \sum_i \frac{\partial \psi}{\partial u_i} \Delta u_i + \frac{1}{2} \sum_i \frac{\partial^2 \psi}{\partial u_i^2} (\Delta u_i)^2 + \sum_{i < j} \frac{\partial^2 \psi}{\partial u_i \partial u_j} \Delta u_i \Delta u_j + \dots \right) d(\Delta \vec{u})$$

For the moments of the velocity increments we write:

$$\langle \Delta u_i \rangle = \int_{-\infty}^{+\infty} \Delta u_i \psi d(\Delta \vec{u}) \quad ; \quad \langle \Delta u_i \Delta u_j \rangle = \int_{-\infty}^{+\infty} \Delta u_i \Delta u_j \psi d(\Delta \vec{u}) \quad (6)$$

The expansion can then be rewritten:

$$W_t \Delta t + \vec{u} \cdot \vec{\nabla} W \Delta t = - \sum_i \frac{\partial W}{\partial u_i} \langle \Delta u_i \rangle + \frac{1}{2} \sum_i \frac{\partial^2 W}{\partial u_i^2} \langle \Delta u_i^2 \rangle - \sum_i W \frac{\partial \langle \Delta u_i \rangle}{\partial u_i} \\ + \sum_i \frac{\partial \langle \Delta u_i^2 \rangle}{\partial u_i} \frac{\partial W}{\partial u_i} + \sum_{i \neq j} \frac{\partial W}{\partial u_i} \frac{\partial \langle \Delta u_i \Delta u_j \rangle}{\partial u_j} + \frac{1}{2} \sum_i \frac{\partial^2 \langle \Delta u_i \rangle}{\partial u_i^2} W \quad (7) \\ + O(\langle \Delta u_i \Delta u_j \Delta u_k \rangle)$$

Keeping terms to first order in Δt , dividing by Δt , and going to the limit of $\Delta t \rightarrow 0$ yields

$$W_t + \vec{u} \cdot \vec{\nabla} W + \vec{\nabla} \cdot (\vec{a} W) + \lim_{\Delta t \rightarrow 0} O\left(\frac{\langle \Delta u_i^2 \rangle}{\Delta t}\right) + \dots = 0 \quad (8)$$

where

$$\vec{a} = \lim_{\Delta t \rightarrow 0} \frac{\langle \Delta \vec{u} \rangle}{\Delta t} \quad (9)$$

Here we consider \vec{a} as a mean acceleration with position \vec{r} , and velocity \vec{u} . Thus the equation of continuity in phase space is

$$W_t + \vec{u} \cdot \vec{\nabla}_r W + \vec{v} \cdot \vec{\nabla}_u (\vec{a} W) = 0 \quad (10)$$

To obtain the continuity equation in configuration space we integrate over velocity space,

$$\rho_t + \vec{v} \cdot (\rho \vec{U}) = 0, \quad (11)$$

where

$$\rho = \int W d\vec{u},$$

and

$$\rho \vec{U} = \int \vec{u} W d\vec{u}.$$

To obtain a momentum equation we multiply the continuity equation in phase space by \vec{u} and integrate over velocity space.

$$(\rho \vec{U})_t + \vec{v} \cdot (\rho \vec{U} \vec{U}) - \rho \vec{A} = 0, \quad (12)$$

where

$$\rho \vec{U} \vec{U} = \int \vec{u} \vec{u} W d\vec{u},$$

and

$$\rho \vec{A} = \int \vec{a} W d\vec{u}.$$

Here \vec{A} is the mean exterior force per unit ρ at \vec{r} , t , and \vec{U} and $\vec{U} \vec{U}$ are the first and second velocity moments respectively of the particles at \vec{r} , t . The continuity equation and the momentum equation now form a hyperbolic system of first order partial differential equations with the dependent variable being the particle density in configuration space. This system of partial differential equations is the diffusion equation in configuration space.

III. INTRODUCTION OF MEAN WIND PROFILE INTO TURBULENCE FIELD

To introduce the mean wind profile into the turbulence field we represent the mean velocity of the diffusing particles as the sum of the mean wind and a macroscopic velocity representative of the turbulent flux with respect to the mean wind field.

$$\vec{U} = \vec{V}(x, y, z) + \vec{v}(x, y, z, t) \quad (13)$$

Furthermore we assume that the velocity in addition possesses a stochastic term which may be represented by a trivariate normal distribution in the components of \vec{u} . This distribution is constructed such as to require that the mean outline of the diffusing particles propagate with a velocity dependent on the stationary wind field independently of time. A distribution satisfying this requirement is

$$W = \frac{1}{(2\pi)^{3/2} |M|^{1/2}} \exp[-1/2 X' M^{-1} X] \cdot \rho(x, y, z, t), \quad (14)$$

where $M = \begin{vmatrix} \mu_{11} & \mu_{12} & \mu_{13} \\ \mu_{21} & \mu_{22} & \mu_{23} \\ \mu_{31} & \mu_{32} & \mu_{33} \end{vmatrix}$, $\mu_{11} = \overline{x_1^2}$, $\mu_{12} = \overline{x_1 x_2}$, etc.

$|M|$ is the determinant of M and X' is the row matrix, $X' = [x_1, x_2, x_3]$, X is the column matrix obtained by transposing X' . We have $x_1 = u_1 - V_1 - v_1$, $x_2 = u_2 - V_2 - v_2$, $x_3 = u_3 - V_3 - v_3$, where the subscripts 1, 2, 3, indicate the components in the i, j, k , directions respectively of $\vec{u}, \vec{V}, \vec{v}$. It is clear that the expected value $\vec{U}\vec{U}$ is

$$\vec{U}\vec{U} = \begin{vmatrix} \mu_{11} \overline{ff} & \mu_{21} \overline{fj} & \mu_{31} \overline{fk} \\ \mu_{21} \overline{jf} & \mu_{22} \overline{jj} & \mu_{23} \overline{jk} \\ \mu_{31} \overline{kf} & \mu_{32} \overline{kj} & \mu_{33} \overline{kk} \end{vmatrix} = \vec{V}\vec{V} + \vec{V}\vec{v} + \vec{v}\vec{V} + \vec{v}\vec{v} + \vec{\sigma}\vec{\sigma}$$

We have defined $\vec{\sigma}\vec{\sigma}$ as the tensor of variances and covariances of velocities relative to the mean $\vec{V} + \vec{v}$.

In this case an assumption that $(\vec{v}\vec{v} + c\vec{c}) = \langle \vec{v}\vec{v} \rangle$ is independent of time gives us the required properties of boundary propagation. We define $\rho\vec{v}$ as the turbulent flux, ξ , and $\rho\langle \vec{v}\vec{v} \rangle$ as the turbulent energy tensor. The substitution of the expressions from equations (13) and (15) into equations (11) and (12) yields

$$\rho_t + \vec{v} \cdot (\rho\vec{V} + \vec{S}) = 0 \quad (16)$$

and

$$(\rho\vec{V} + \vec{S})_t + \vec{v} \cdot [\rho\vec{V}\vec{V} + \vec{S}\vec{V} + \vec{V}\vec{S} + \rho\langle \vec{v}\vec{v} \rangle] - \rho\vec{A} = 0. \quad (17)$$

The above equations constitute a hyperbolic system of first order partial differential equations. These equations describe the transfer of a scalar quantity, through a turbulent fluid. Particulate diffusion and heat transfer are processes for which the equations should hold.

We now seek to relate \vec{A} and $\langle \vec{v}\vec{v} \rangle$ to measurable quantities. Once \vec{A} and $\langle \vec{v}\vec{v} \rangle$ are given, it is clear that with the four equations (one from the continuity equation) (16), and the three from the vector momentum equation (17), and the four unknowns (ρ and the three components of \vec{S}), Cauchy initial data is sufficient to determine the hyperbolic system of equations (16) and (17) [2].

For \vec{A} we choose an acceleration caused by a resistive force which is proportional to the turbulent flux in each direction and an external force term which reflects the contribution of gravity-buoyancy effects in the case of heavy particles.

$$\vec{A}_p = - [i_\alpha(i \cdot \vec{S}) + j_\beta(j \cdot \vec{S}) + k_\gamma(k \cdot \vec{S})] + \vec{c}_p \quad (18)$$

The resistive force coefficient is interpreted as the probability per unit time of reversal of the diffusing particle. Monin [18], Davies [8], and Goldstein [13] independently derive similar expressions. We are assuming that there is no resistance to the mean flow, \vec{V} .

Kazanskii and Monin report satisfactory experimental verification of a similarity theory application using the same resistance term [15] [21]. Monin interprets the resistance term as being equivalent to a typical frequency of pulsation of the turbulence. Monin's approach seems consistent with the present development. The values of this term may be deduced experimentally from steady state evaluations of the concentrations.

For the turbulent energy tensor, $\langle \vec{v}\vec{v} \rangle$, we propose that the Reynolds stress tensor be used. We propose that the second velocity moment of the diffusing particles, with respect to the mean wind field, is locally proportional to that of the turbulent fluid. At present, for simplicity and heuristic purposes, the proportionality constant will be assumed as unity. Experiments such as smoke puff and plume outline photography may determine more appropriate proportionality coefficients. It must be kept in mind that careful consideration of the type of averaging used in representing $\langle \vec{v}\vec{v} \rangle$ is germane to any application. The $\langle \vec{v}\vec{v} \rangle$ averaging must be compatible with the averaging used to determine \bar{V} .

Equation (17) then becomes

$$(\rho \vec{v} + \vec{S})_t + \vec{v} \cdot [\rho \vec{v}\vec{v} + \vec{S}\vec{v} + \vec{v}\vec{S} + \rho \langle \vec{v}\vec{v} \rangle] + \quad (19)$$

$$\hat{i}_a(\hat{i} \cdot \vec{S}) + \hat{j}_a(\hat{j} \cdot \vec{S}) + \hat{k}_a(\hat{k} \cdot \vec{S}) - \vec{c}\rho = 0.$$

Formally to obtain \vec{A} we could have stated similarly to the Kramers - Chandrasekhar approach to Brownian motion in a field of force [1]. The increment of velocity, $\Delta \vec{u}$, which the particle experiences in the time Δt is expressed as the sum of a term due to the external field of force, $\vec{K}\Delta t$, and a fluctuating quantity with a given law of distribution, $\vec{B}(\Delta t)$.

$$\Delta \vec{u} = \vec{K}\Delta t + \vec{B}(\Delta t). \quad (20)$$

The classical distribution of $\vec{B}(\Delta t)$ is given by

$$w(\vec{B}[\Delta t]) = \frac{1}{(4\pi q \Delta t)^{3/2}} e^{(-|\vec{B}(\Delta t)|^2 / 4q \Delta t)} \quad (21)$$

where

$$q = \beta kT/m.$$

Physically, $\vec{B}(\Delta t)$ represents the net acceleration which a particle experiences in time Δt under the influence of molecular scale fluctuations. We shall neglect it compared to the much larger scale of turbulence fluctuations. Thus δ also reduces to the Dirac delta function, $\delta(\Delta u - \vec{K} \Delta t)$. For the term \vec{K} we propose a frictional force acting on the diffusing particle proportional to the turbulent flux velocity and external force per unit ρ due to buoyancy-gravity effects.

$$\vec{K} = - [\hat{i}\alpha(\hat{i}\cdot\vec{v}) + \hat{j}\delta(\hat{j}\cdot\vec{v}) + \hat{k}\gamma(\hat{k}\cdot\vec{v})] + \vec{c} \quad (22)$$

Substituting these values into equation (4) we may formally obtain equations (16) and (19).

IV. NORMALIZATION

In any application of the hyperbolic diffusion equation it must be remembered that ρ is a probability density. Hence the concentration must be normalized. If the equation were parabolic, a single term would be sufficient to normalize the concentration. However, for the hyperbolic equation it is necessary to perform two integrations to normalize, one over the characteristic surfaces, and one over the volume contained therein. Davies discusses this procedure [8].

V. THE CHARACTERISTIC SURFACES

The characteristic surfaces of the hyperbolic diffusion equation provide a useful parameter of the effectiveness of diffusion. The characteristics of the hyperbolic diffusion equation are the loci of points of discontinuity of the atmospheric contaminant. All solutions exist within the characteristics; there is no concentration outside of the characteristics. The characteristics in effect represent wave fronts of the diffusing particles.

Pasquill [25] finds that the vertical spread of diffusing particles in a parabolic Lagrangian similarity treatment is best represented by an extreme height encompassing most of the particles, essentially as in the hyperbolic treatment of Monin. In the present hyperbolic model this concept is intrinsic rather than arbitrary as in the parabolic equation application. The extremum corresponds to the characteristics of the hyperbolic equation.

VI. THE PARABOLIC DIFFUSION EQUATION AS A LIMITING FORM OF THE HYPERBOLIC EQUATION

Using a method similar to Davies [8], [9], and Monin [18], the parabolic diffusion equation will be derived from the hyperbolic diffusion equation. The momentum equation may be written

$$((\rho \vec{V} + \vec{S})_t + \vec{\nabla} \cdot [\rho \vec{V}\vec{V} + \vec{S}\vec{V} + \vec{V}\vec{S} + \rho \langle \vec{v}\vec{v} \rangle]) + \hat{i}\alpha(\hat{i} \cdot \vec{S}) + \hat{j}\delta(\hat{j} \cdot \vec{S}) + \hat{k}\gamma(\hat{k} \cdot \vec{S}) - \hat{e}\rho = 0$$

$$\begin{vmatrix} \frac{1}{\alpha} \hat{i}\hat{i} & 0 & 0 \\ 0 & \frac{1}{\delta} \hat{j}\hat{j} & 0 \\ 0 & 0 & \frac{1}{\gamma} \hat{k}\hat{k} \end{vmatrix} = 0 \quad (23)$$

If $1/\alpha$, $1/\delta$, $1/\gamma$, are considered as parameters, and the following limits are said to exist,

$$\{(\hat{i} + \hat{j} + \hat{k}) \cdot \langle \vec{v}\vec{v} \rangle\} \cdot \begin{vmatrix} \frac{1}{\alpha} \hat{i}\hat{i} & 0 & 0 \\ 0 & \frac{1}{\delta} \hat{j}\hat{j} & 0 \\ 0 & 0 & \frac{1}{\gamma} \hat{k}\hat{k} \end{vmatrix} \lim_{\alpha, \delta, \gamma} = [K]_1 \hat{i} + [K]_2 \hat{j} + [K]_3 \hat{k} \quad (24)$$

$$\{\vec{\nabla} \cdot \langle \vec{v}\vec{v} \rangle\} \cdot \begin{vmatrix} \frac{1}{\alpha} \hat{i}\hat{i} & 0 & 0 \\ 0 & \frac{1}{\delta} \hat{j}\hat{j} & 0 \\ 0 & 0 & \frac{1}{\gamma} \hat{k}\hat{k} \end{vmatrix} \lim_{\alpha, \delta, \gamma} = v_1 \hat{i} + v_2 \hat{j} + v_3 \hat{k} \quad (25)$$

$$\hat{e} \cdot \begin{vmatrix} \frac{1}{\alpha} \hat{i}\hat{i} & 0 & 0 \\ 0 & \frac{1}{\delta} \hat{j}\hat{j} & 0 \\ 0 & 0 & \frac{1}{\gamma} \hat{k}\hat{k} \end{vmatrix} \lim_{\alpha, \delta, \gamma} = v_{e1} \hat{i} + v_{e2} \hat{j} + v_{e3} \hat{k} \quad (26)$$

limits: $\lim \langle \vec{v}\vec{v} \rangle \rightarrow$
 $\lim \alpha, \delta, \gamma \rightarrow$
 $\lim \vec{\nabla} \cdot \langle \vec{v}\vec{v} \rangle \rightarrow$
 $\lim \hat{e} \rightarrow$ 12

then, taking the limits and substituting the momentum equation into the continuity equation, a parabolic diffusion equation is found.

$$\frac{\partial \rho}{\partial t} = - \sum_{i=1}^3 \frac{\partial}{\partial r_i} [V_{D1}(\vec{r}) \rho] + \sum_{k,l=1}^3 \frac{\partial}{\partial r_k} [K_{k,l}(\vec{r}) \frac{\partial \rho}{\partial r_l}] \quad (27)$$

where $V_{D1} = V_1 - v_1 + v_{e1}$

Essentially we have the hyperbolic equation going to the parabolic equation after times very large compared to $\frac{1}{v}$, $\frac{1}{v}$. The parabolic diffusion equation found above is the three dimensional Fokker-Planck equation [29] [30]. If $\vec{V} = V(z)\hat{i}$ and $\langle \vec{v}\vec{v} \rangle$ has no diagonal terms, equivalent to partition of energy in the i, j, k, directions, then we have the semi-empirical parabolic diffusion equation for the lower atmosphere [20] [24]. If in addition $\vec{V}_D = 0$, the Smoluchowski equation is obtained [1].

VII. FUTURE DEVELOPMENT

→ In the case of constant mean velocity, and isotropic $\langle v v \rangle$, the present model reduces to those of Davies [8], Goldstein [13], and Monin [18] in the appropriate number of spatial dimensions. It is not fully clear under what conditions the models are consistent with the various spectra. In addition the effects of meandering have not been included. Further refinement and development of the present model, especially with respect to spectra and pair particle density consideration, may be fruitful along the phase space approach of Tchen [29] and the statistical representation of meandering by Gifford [11] [12]. These approaches are consistent with the development of the present model. The role of large and small eddy scales may then be explicitly included.

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13. ABSTRACT A three dimensional hyperbolic differential equation based on finite correlated particle velocities is derived which is appropriate to modeling anisotropic turbulent diffusion in the atmosphere. Cauchy initial data, the mean wind, the Reynolds stress tensor, and a typical frequency of pulsation are required for complete solution. The outlines of plumes and puffs may be obtained with only knowledge of the Reynolds stress tensor and mean wind velocity. The classical parabolic diffusion equations are a limiting form of this hyperbolic Δt .		

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Security Classification

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14.	KEY WORDS	LINK A		LINK B		LINK C	
		ROLE	WT	ROLE	WT	ROLE	WT
	Atmospheric Diffusion Turbulent Diffusion Hyperbolic Diffusion Equation Parabolic Diffusion Equation Hyperbolic Differential Equation Phase Space Markov Process in Phase Space Diffusion Particle Diffusion						
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