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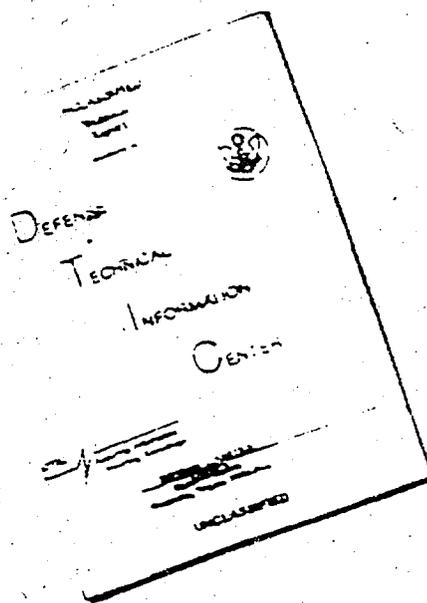
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OF THE EQUATION  
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SOME LIMITATIONS ON THE FORM OF THE EQUATION  
OF ATMOSPHERIC DIFFUSION

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Program Coordination Office

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ABSTRACT

Some simple transformation properties of the diffusion equation that has been classically used to describe turbulent transport in the atmosphere are briefly examined. The essential tensorial nature of the eddy diffusivity is emphasized, and it is concluded that the standard form frequently adopted for the diffusion equation in the meteorological literature cannot be generally valid.

## I. INTRODUCTION

We consider the equation that is frequently quoted in the meteorological literature as describing the turbulent diffusion of a conservative scalar property in three dimensions. For present purposes the density of the fluid medium will be supposed to be constant, and the standard general form of the equation taken to be<sup>1-4</sup>

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = \frac{\partial}{\partial x} \left( K_1 \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_2 \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_3 \frac{\partial C}{\partial z} \right) \quad (1)$$

relative to a fixed system of rectangular Cartesian coordinates  $Oxyz$ . Here  $C = C(x, y, z, t)$  is a suitably defined mean concentration;  $u, v, w$  are the mean velocity components of the fluid motion;  $K_1, K_2, K_3$  are the so-called eddy diffusion coefficients, which are assumed to be functions of position. Unfortunately the precise nature of the quantities  $K_1, K_2,$  and  $K_3$  (e.g., whether they are scalar functions of position or components of a vector function, etc.) is rarely discussed in the meteorological contexts. Since this question is vital to the interpretation of the equation it is briefly examined in this manuscript. It is shown that, even under the customary assumptions, Equation (1) cannot be a generally valid form of diffusion equation.

## II. A GENERAL TRANSFORMATION

More fundamentally, the right side of Equation (1) is the negative of  $\text{div } \underline{F} \equiv \partial F_x / \partial x + \partial F_y / \partial y + \partial F_z / \partial z$  where  $\underline{F} = (F_x, F_y, F_z)$  is the turbulent flux vector for the scalar property considered. Equation (1) then results from the hypothesis that the components of  $\underline{F}$  relative to the axes  $Oxyz$  are related in a simple homogeneous linear fashion to the respective components of the concentration gradient vector  $\partial C / \partial \underline{x} \equiv (\partial C / \partial x, \partial C / \partial y, \partial C / \partial z)$ .

Let the Greek symbols  $\alpha, \beta, \gamma,$  etc. stand for any of  $x, y,$  or  $z,$  and let us define for the chosen axes  $Oxyz$  an ordered array of nine quantities  $K_{\alpha\beta}$  by the matrix equation

$$K_{\alpha\beta} \equiv \begin{pmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{pmatrix} = \begin{pmatrix} K_1 & 0 & 0 \\ 0 & K_2 & 0 \\ 0 & 0 & K_3 \end{pmatrix} \quad (2)$$

For convenience we shall also use the Einstein summation convention, according to which, in any term containing a repeated Greek suffix, it is understood that the suffix is given all possible values  $x, y, z$  and

the terms so obtained are then added. Then at any chosen point of the medium Equation (1) is exactly equivalent to the following relation between the components of  $\underline{F}$  and those of  $\frac{\partial C}{\partial r}$ :

$$F_{\alpha} = - K_{\alpha\beta} \frac{\partial C}{\partial r_{\beta}} \quad (3)$$

We now consider a second arbitrary set of rectangular axes  $Ox'y'z'$ , and let  $t_{\alpha\beta'}$  denote the cosine of the angle between the axes  $O\alpha$  and  $O\beta'$ , so that  $t_{\alpha\beta'} = t_{\beta'\alpha}$ . Then the components of the vector  $\underline{F}$  relative to the new axes will be given by

$$F_{\gamma'} = F_{\alpha} t_{\alpha\gamma'} \quad (4)$$

Similarly, the components of the gradient vector  $\frac{\partial C}{\partial r}$  for the axes  $Oxyz$  will be related to those for the axes  $Ox'y'z'$  by

$$\frac{\partial C}{\partial r_{\beta}} = \frac{\partial C}{\partial r_{\delta'}} t_{\delta'\beta} \quad (5)$$

From Equations (3), (4), and (5) it follows that

$$\begin{aligned} F_{\gamma'} &= - K_{\alpha\beta} \frac{\partial C}{\partial r_{\beta}} t_{\alpha\gamma'} = - K_{\alpha\beta} \frac{\partial C}{\partial r_{\delta'}} t_{\delta'\beta} t_{\alpha\gamma'} \\ &= - K_{\alpha\beta} \frac{\partial C}{\partial r_{\delta'}} t_{\alpha\gamma'} t_{\beta\delta'} \end{aligned} \quad (6)$$

Equation (6) provides the rule for relating the components of the flux vector  $\underline{F}$  and the gradient vector  $\frac{\partial C}{\partial r}$  in the new axes  $Ox'y'z'$ . It may equivalently be written

$$F_{\gamma'} = - K_{\gamma'\delta'} \frac{\partial C}{\partial r_{\delta'}} \quad (7)$$

where

$$K_{\gamma'\delta'} = K_{\alpha\beta} t_{\alpha\gamma'} t_{\beta\delta'} \quad (8)$$

Equation (8), however, defines the known transformation law for a second-order Cartesian tensor.<sup>6</sup> It thus establishes the fact that the set of quantities  $K_{\alpha\beta}$  in Equation (2) constitute the components of a second-order tensor. This is a direct consequence of the vectorial nature of  $\underline{F}$  and  $\frac{\partial C}{\partial r}$ . The tensor  $K_{\alpha\beta}$  is, of course, in general a function of position, since the relation between  $\underline{F}$  and  $\frac{\partial C}{\partial r}$  will be defined at every point of the medium. We see from Equation (7) that in the arbitrary axes  $Ox'y'z'$  the components of  $\underline{F}$  are general homogeneous linear functions of the components of  $\frac{\partial C}{\partial r}$ . This relationship is exactly analogous to that encountered in considering molecular heat conduction in an anisotropic medium. Whether such a linearity hypothesis is actually justified for the

turbulent flux of a scalar property can, of course, only be decided on the basis of experiment. For any physical meaning to be attached to the tensor  $K_{\alpha\beta}$  (or  $K_{\alpha\beta}$ ), it is evident that it must be a property of the fluid motion, i.e., independent of the distribution of the diffusing scalar property. We may call  $K_{\alpha\beta}$  the eddy diffusivity tensor.

It may be noted that the requirement for such a tensor quantity is actually suggested by an obvious extension of the Prandtl mixing-length concept to three dimensions. Thus, if we suppose that the turbulent fluctuation of concentration  $C'$  from the mean value  $C$  is given by

$$C' = - \underline{l} \cdot \frac{\partial C}{\partial \underline{r}} = - l_{\beta} \frac{\partial C}{\partial r_{\beta}}$$

so that  $\underline{l} = (l_x, l_y, l_z)$  is the mixing-length vector, then if  $V_{\alpha}'$  denotes a component of the turbulent velocity fluctuation, and an overbar denotes a mean value,

$$\begin{aligned} F_{\alpha} &= \overline{V_{\alpha}' C'} = - \overline{V_{\alpha}' l_{\beta}} \frac{\partial C}{\partial r_{\beta}} \\ &= -K_{\alpha\beta} \frac{\partial C}{\partial r_{\beta}} \quad \text{where} \quad K_{\alpha\beta} = \overline{V_{\alpha}' l_{\beta}} \end{aligned}$$

and  $K_{\alpha\beta}$  is clearly a second-order tensor.

Relative to the axes  $Ox'y'z'$  the right side of Equation (1), which represents  $-\text{div } \underline{E}$ , is replaced by the nine-term sum represented under the summation convention by

$$\frac{\partial}{\partial r_{\alpha}'} \left( K_{\alpha'\beta'} \frac{\partial C}{\partial r_{\beta}'} \right)$$

### III. SOME SPECIAL FORMS

The special diagonal form of the tensor  $K_{\alpha\beta}$  in Equation (2) relative to the axes Oxyz implies that at the chosen point of the medium the diffusivity tensor is symmetric (since symmetry is a property preserved under transformation of axes, and  $K_{\alpha\beta}$  is clearly symmetric) and further that Oxyz are its principal axes. For Equation (1) to be valid at all points of the medium it would also be necessary for the tensor to have Oxyz as principal axes at all points of space. It therefore follows that Equation (1) cannot be adopted as a possible general form of diffusion equation because the axes Oxyz cannot be chosen arbitrarily but must be a preferred set with the above properties. A special case would arise if the (symmetric) diffusivity tensor were isotropic at all points of the medium, i.e., if  $K_1 = K_2 = K_3 = \text{say } k$  (a scalar function of position) so that

$$K_{\alpha\beta} = k \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

In this case its components would be the same for all rectangular axes and all axes would be principal axes. Then from Equation (3), the flux vector would be

$$\underline{F} = -k \frac{\partial C}{\partial \underline{r}}$$

and the corresponding diffusion equation

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = \frac{\partial}{\partial x} \left( k \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial C}{\partial z} \right) \quad (9)$$

For this special isotropic form of diffusion equation there are no preferred axes.

Having recognized the above fundamental limitations on the use of Equation (1) we may seek for a meteorological situation where it might appear plausible to postulate the existence of a preferred set of axes, independent of spatial location. Such a situation could occur in the surface layers of the atmosphere, where the mean wind vector can be regarded approximately as everywhere parallel to a given vertical plane. This uniquely defined vertical plane, together with the vertical direction (which must be fundamental to the characteristics of turbulence generated by the horizontal ground surface) will suffice to define a preferred set of axes, e.g., Ox and Oz in the plane and, respectively, horizontal and vertical; and Oy perpendicular to the plane, i.e., perpendicular to the mean velocity vector. Relative to these axes the mean velocity component  $v$  of Equation (1) is  $v = 0$ . If it is postulated that this preferred set

of axes is a principal set for a symmetric diffusivity tensor at every point of the medium, then relative to this special set of axes the diffusion equation would have the form

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + w \frac{\partial C}{\partial z} = \frac{\partial}{\partial x} \left( K_1 \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_2 \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_3 \frac{\partial C}{\partial z} \right) \quad (10)$$

where  $K_1$ ,  $K_2$ , and  $K_3$  are scalar functions of position that define the principal components of the diffusivity tensor. For the situation visualized above, it is also normally assumed that the vertical component of mean velocity  $w = 0$ . Of course, whether such a set of stringent postulates does correspond to the real atmospheric diffusion process can only be justified on the basis of experiment.

It should be emphasized that the possible existence of a preferred set of axes in the above example depends on the assumption that the mean velocity vector is everywhere parallel to a given vertical plane, so that a preferred set of horizontal axes can be defined (since we have already assumed that the vertical direction is a preferred one). If this assumption were not made, for example, if we were to assume<sup>3</sup> only that the mean velocity was parallel to the ground surface with general components  $u \neq 0$ ,  $v \neq 0$ ,  $w = 0$ , then no preferred horizontal axes  $Ox$ ,  $Oy$  could be defined, and hence a diffusion equation of the form  $(K_1 + K_2)$

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = \frac{\partial}{\partial x} \left( K_1 \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_2 \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_3 \frac{\partial C}{\partial z} \right) \quad (11)$$

would not be valid. This form of equation could only be valid in the special case  $K_1 = K_2$ , i.e., if the tensor quadric had rotational symmetry about the  $z$  axis.

Finally, it should be noted that, although the above discussion has been restricted to rectangular axes for reasons of simplicity, the questions raised will be quite fundamental when considering possible forms for the equation of turbulent diffusion in other coordinate systems, e.g., any system of orthogonal curvilinear coordinates. For such cases it will be necessary to apply the methods of general tensor analysis.

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