Solutions of Diffusion-Advection Problems by Ray Methods

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ABSTRACT

An asymptotic procedure utilizing ray methods is applied to the problem of dispersion from an instantaneous point source under the combined influence of diffusion and advection. It is found that the ray method offers a relatively simple procedure for obtaining a first asymptotic approximation to the solution. In certain instances, the first approximation turns out to be the exact solution, while in the remaining cases, somewhat more work will yield a full asymptotic expansion.

In two particular cases, the exact solution is obtained with the help of these methods. In the first case, the flow velocities are any linear combination of the coordinates, and the diffusion coefficients are arbitrary constants. The other case is a one-dimensional problem without advection, but in which the diffusion coefficient is a linear function of height.

1. INTRODUCTION

In recent years, attention has been drawn to the importance of advection as well as diffusion in problems of dispersion in a fluid (Okuba, 1968), (Bowles et al, 1958), (Bowden, 1965). Thus, when an experiment is performed involving the release of dye, say to estimate a turbulent diffusion coefficient, the shear in the fluid motion increases the dispersion of the dye beyond the amount to be expected from diffusion alone.

In order to estimate this effect, solutions of the diffusion advection equation are required for various flow patterns. Under certain circumstances, this may be done with Fourier Transform methods, but direct application of these methods can involve serious difficulties (Neuringer, 1968) even with simple flow patterns. For this reason, solutions that have appeared to date (Okuba, 1968), (Neuringer, 1968) usually correspond to the simple case of linear shear in one direction, plus minor variations such as a constant gravitational field or a time-dependent and space-independent mean flow.

However, it is often the case that an asymptotic solution, rather than an exact solution, is sufficient to obtain qualitative and even quantitative features of the solution, and asymptotic methods are frequently easier to apply. A particularly powerful procedure has been developed by J. B. Keller (Keller, 1958), (Keller, 1962), for application to various wave problems, and later extended

by R. M. Lewis (Lewis and Keller, 1963), (Lewis, 1964), (Cohen and Lewis, 1967) to a variety of other problems. These problems include optics (Keller, 1962), acoustics (Jeffreys, 1962), water waves (Keller, 1958), (Shen and Meyer, 1967) as well as isotropic diffusion without advection (Cohen and Lewis, 1967).

The central feature of this technique is the construction of approximate solutions by the use of rays, that is, a family of curves in space-time on which the approximate solutions satisfy ordinary differential equations. The rays are themselves defined with ordinary differential equations, which are generally simpler to deal with than the original partial differential equations.

In the present paper, we apply the Keller-Lewis ray theory to the problem of anisotropic diffusion-advection, and consider specifically the case of an instantaneous point source. In the course of so doing, we obtain an extra dividend: for a wide class of flows, the ray technique leads, not to a sequence of approximate solutions, but to the exact solution itself.

In §§2-4 of the paper, we develop the formal ray method procedures. In section 2, we introduce a "large parameter" into the equation, that is, a scaling factor relating the diffusion coefficients to other scales in the problem. We then write the solution formally as an asymptotic expansion in this parameter and obtain first order partial differential equations which the various terms in the expansion must satisfy.

In section 3, it is seen that the differential equations for the terms of the asymptotic expansion lead to the formulation of ordinary differential equations for the rays, and the value of each time in the asymptotic expansion for each ray of the family.

In section 4, we obtain boundary conditions for our rays in terms of the boundary conditions for the diffusion equation itself.

In section 5, the ray methods are used to solve several particular examples. First is the diffusion in two dimensions through a linear shear flow, as considered by (Neuringer, 1968). The asymptotic expansion truncates, and the exact solution is found to be the first term in the expansion.

Our second example generalizes the first to the case where the velocities u_i are arbitrary linear functions of the coordinates, whose coefficients, together with the diffusion coefficients K_{ij}, are arbitrary continuous functions of time. Special cases include diffusion in three dimensions through a linear shear flow, as considered by (Okuba, 1968), as well as bilinear shear flows in two dimensions.

The final example solves the problem of one-dimensional diffusion without advection, in which the diffusion coefficient is linear with distance. In this case, the ray method leads us to an asymptotic expansion for the exact solution. Indeed, although the asymptotic expansion converges nowhere, its form turns out to be sufficient

clue to determine the exact solution, and it is then easy to verify the above statement that the ray expansion is asymptotic to the solution.

In sections 2-4, we shall generally use ~~$\hat{x}_i$~~ x_i for the position coordinates, u_i for the velocity component, and K_{ij} for the coefficients of diffusion. We shall use the summation convention that, whenever a subscript appears twice in a single term, we assume summation over the subscript from 1 to N where N denotes the number of dimensions under consideration.

§2. The Diffusion, Dispersion, and Transport Equations

We assume in this paper that anisotropic diffusion in a fluid medium is governed by the equation

$$\frac{\partial C}{\partial \hat{t}} + \frac{\partial}{\partial \hat{x}_i}(\hat{u}_i C) = \frac{\partial}{\partial \hat{x}_i}\left(\hat{K}_{ij}\frac{\partial C}{\partial \hat{x}_j}\right) \qquad (2.1)$$

wrong form
for divergent flows.

in which the diffusion coefficients $\hat{K}_{ij}(\hat{x}_i, \hat{t})$ form a symmetric, positive definite tensor, and together with the velocity components $\hat{u}_i(\hat{x}_i, \hat{t})$, are prescribed, continuously differentiable functions of position $\hat{x}_i$ and time $\hat{t}$. Except for the concentration C itself all dimensional quantities are denoted with a superposed cap " ^ ".

These assumptions suffice to ensure that an initial-boundary value problem on a compact domain, with C specified both initially and on the boundary, is well posed. Furthermore, for a problem in an unbounded domain uniqueness results from a "radiation condition" of this type:

$$\hat{u}_i\, C^2 = o\left(\frac{1}{\hat{r}^{N-1}}\right), \quad \hat{K}_{ij}\, C\,\frac{\partial C}{\partial \hat{x}_j} = o\left(\frac{1}{\hat{r}^{N-1}}\right) \quad \text{as } \hat{r}\to\infty \tag{2.2}$$

where $\hat{r}^2 = \hat{x}_i\,\hat{x}_i$, N denotes the number of dimensions, and o denotes /l.c.
"small order of", i. e. $\hat{r}^{N-1}\,\hat{u}_i\, C^2 \to 0$.

Our concern in the present paper will lie in the "Green's Function" or "instantaneous point source" problem. Locating the instantaneous point source at the origin at time zero requires the condition

$$C(\hat{x}_i, \hat{t}) \longrightarrow S\,\delta(\hat{x}_i) \quad \text{as } t\downarrow 0 \tag{2.3}$$

where $\delta(\hat{x}_i)$ denotes the Di/ac delta function of $\hat{x}_i$, and S denotes /r
the source strength.

By (2.3) is meant the relation

$$\int C(\hat{x}_i, \hat{t})\,\varphi(\hat{x}_i)\,d\hat{x}_i \longrightarrow \varphi(0) \quad \text{as } t\downarrow 0$$

for all bounded, indefinitely differentiable functions φ .

This implies, in particular,

$$\int C(\hat{x}_i, \hat{t})\,d\hat{x}_i \longrightarrow S \quad \text{as } t\downarrow 0$$

$$C(\hat{x}_i, \hat{t}) \longrightarrow 0 \quad \text{as } t\downarrow 0 \quad \text{for } \hat{r}\neq 0$$

We introduce non-dimensional variables

$$\begin{aligned} x_i &= \hat{x}_i/L \\ t &= \hat{t}/T \\ K_{ij} &= \hat{K}_{ij}/\Psi \\ u_i &= \hat{u}_i\, T/L \end{aligned} \tag{2.4}$$

where L, T and Ψ denote "typical" values of length, time, and diffusion coefficient, respectively.

Then (2.1) and (2.3) become

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x_i}(u_i C) = \frac{1}{\lambda}\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial C}{\partial x_j}\right) \tag{2.5}$$

$$C(x_i, t) \longrightarrow S\,L^N\,\delta(x_i) \quad \text{as } t\downarrow 0 \tag{2.6}$$

where $\lambda = \frac{L^2}{\Psi T}$. Without loss of generality, we may take SL^N to be unity.

The (non-dimensional) parameter λ in (2.5) is precisely the "large parameter" in which we seek asymptotic approximations to the solution. We will be interested in the behavior of solutions of (2.5) as $\lambda\to\infty$. The meaning of this limit may be visualized as concerning larger and larger length scales, or smaller and smaller time scales and/or diffusion coefficients.

Following the Keller-Lewis ray procedure, we apply one of the following forms of "Ansatz"

$$C(x_i, t) = A(x_i, t;\lambda)\, e^{\lambda\psi(x_i,t)} \tag{2.7a}$$

or

$$C(x_i, t) \approx e^{\lambda\psi(x_i,t)} \sum A^{(n)}(x_i, t)\,\lambda^{-n+\alpha} \quad \text{as } \lambda\longrightarrow\infty \tag{2.7b}$$

The original use of the form (2.7a) seems to be due to Sommerfield and Runge (Kline and Kay, 1965), while the form (2.7b) is more generally used in the Keller-Lewis theory.

The motivation for (2.7) lies, first in the form of the well-known exact solution for (2.5), (2.6) for isotropic stationary media:

$$C(x_i, t) = \left(\frac{\lambda}{4\pi K t}\right)^{n/2} \exp\left(-\lambda \frac{x_i x_i}{4Kt}\right)$$

and secondly in the success in applying "Ansatze" similar to (2.7) to acoustics and geometrical optics. In the latter cases, the $\lambda\psi$ in the exponential functions is replaced by $i\lambda\varphi$.

To define the functions $\psi, A, A^{(n)}$, we substitute (2.7) directly in (2.5). The result is an expansion in powers of λ whose coefficients are expressions involving $\psi, A, A^{(n)}$.

By setting each such coefficient to zero, we obtain the following equations:

$$\frac{\partial \psi}{\partial t} + u_i \frac{\partial \psi}{\partial x_i} = K_{ij} \frac{\partial \psi}{\partial x_i} \frac{\partial \psi}{\partial x_j} \qquad (2.8)$$

and

$$\frac{\partial A}{\partial t} + \frac{\partial}{\partial x_i}(u_i A) = \frac{1}{\lambda} \frac{\partial}{\partial x_i}\left(K_{ij} \frac{\partial A}{\partial x_j}\right) + 2K_{ij} \frac{\partial A}{\partial x_i} \frac{\partial \psi}{\partial x_j} + A \frac{\partial}{\partial x_i}\left(K_{ij} \frac{\partial \psi}{\partial x_j}\right) \qquad (2.9)$$

for (2.7a), or

$$\frac{\partial A^{(0)}}{\partial t} + \frac{\partial}{\partial x_i}(u_i A^{(0)}) = 2K_{ij} \frac{\partial \psi}{\partial x_i} \frac{\partial A^{(0)}}{\partial x_j} + A^{(0)} \frac{\partial}{\partial x_i}\left(K_{ij} \frac{\partial \psi}{\partial x_j}\right) \qquad (2.10a)$$

$$\frac{\partial A^{(n)}}{\partial t} + \frac{\partial}{\partial x_i}(u_i A^{(n)}) = 2K_{ij} \frac{\partial \psi}{\partial x_i} \frac{\partial A^{(n)}}{\partial x_j} + A^{(n)} \frac{\partial}{\partial x_i}\left(K_{ij} \frac{\partial \psi}{\partial x_j}\right) + \frac{\partial}{\partial x_i}\left(K_{ij} \frac{\partial A^{(n-1)}}{\partial x_j}\right) \qquad (2.10b)$$

for (2.7b)

In the case of geometric optics and acoustics, the function φ corresponding to ψ is related to Brun's eiconal (Kline and Kay, 1965), and the analogue of (2.8) is known as the eiconal equation. In the present case, this name is inappropriate since the behavior of solutions of (2.8) is significantly different from those of the eiconal equation. Accordingly, we follow Lewis in calling (2.8) the <u>dispersion equation</u>.

The equations (2.10), with which we will be working, are known as the <u>transport equations</u> and the $A^{(n)}$ as the <u>transport terms</u>. These equations define the transport terms iteratively, using and $A^{(n-1)}$ to obtain $A^{(n)}$. As will be seen, a constructive procedure exists for the solution of (2.8) - (2.10). When these terms are obtained, the expansion (2.7b) may be expected to yield an asymptotic expansion to the solution.

The equations (2.7a) and (2.9), on the other hand, may be found useful on occasion in obtaining or verifying an exact solution (see section 5). However, the constructive procedure developed for (2.10) does not work for (2.9).

3. The Ray Method

The dispersion and transport equations (2.8) and (2.10) of the last section are both equations of the first order. But it is known (Courant and Hilbert, 1962), (Garabedian, 1964) that whenever such equations have a solution, the solution may be obtained by the method of characteristics.

If we set $\quad p_i = \frac{\partial \psi}{\partial x_i}, \quad s = \frac{\partial \psi}{\partial t}$

the dispersion equation (2.8) becomes

$$s + u_i p_i = K_{ij} p_i p_j \tag{3.1}$$

and the characteristic equations are

$$\begin{aligned}
\frac{dx_i}{d\sigma} &= \mu\left[u_i - 2K_{ij} p_j\right] \\
\frac{dt}{d\sigma} &= \mu \\
\frac{d\psi}{d\sigma} &= \mu\left[s + u_i p_i - 2K_{ij} p_i p_j\right] \\
\frac{dp_i}{d\sigma} &= -\mu\left[\frac{\partial u_j}{\partial x_i} p_j - \frac{\partial K_{j\ell}}{\partial x_i} p_j p_\ell\right] \\
\frac{ds}{d\sigma} &= -\mu\left[\frac{\partial u_j}{\partial t} p_j - \frac{\partial K_{j\ell}}{\partial t} p_j p_\ell\right]
\end{aligned} \tag{3.2}$$

If a solution $\psi(x_i, t)$ has, at a point x_i° at time t^o, the value ψ°, and the derivatives $\frac{\partial \psi}{\partial x_i}$, $\frac{\partial \psi}{\partial t}$ have values p_i°; s° respectively, this poses an initial value problem for (3.2). The solution of this problem yields a trajectory, $x_i(\sigma), t(\sigma)$ in parametric representation, and everywhere on this trajectory $\psi(\sigma)$, $p_i(\sigma)$ and $s(\sigma)$ agree with $\psi(x_i, t)$, $\frac{\partial \psi}{\partial x_i}(x_i, t)$, and $\frac{\partial \psi}{\partial t}(x_i, t)$.

The arbitrary proportionality factor $\mu(\sigma)$ may be selected to use any quantity which increases monotonically along the trajectory as the parameter σ. In particular, setting $\mu = 1$ allows us to identify $\sigma = t$.

It is known that if the initial values $s^\circ, p_i^\circ, x_i^\circ$ and t^o satisfy (3.1), then the solution to (3.2) will satisfy (3.1) identically.

Accordingly, we may subtract (3.1) from the formula for $\frac{d\psi}{d\sigma}$ in (3.2). Making these changes, we find that (3.2) reduces to:

$$\left.\begin{aligned}
\frac{dx_i}{dt} &= u_i - 2K_{ij} p_j \\
\frac{d\psi}{dt} &= -K_{ij} p_i p_j \\
\frac{dp_i}{dt} &= -\frac{\partial u_j}{\partial x_i} p_j + \frac{\partial K_{j\ell}}{\partial x_i} p_j p_\ell
\end{aligned}\right\} \tag{3.3}$$

We have dropped the equation for $\frac{ds}{dt}$ since it is no longer needed to form a well-defined problem.

In the general theory of first order partial differential equations, the solution of (3.3) (or (3.2)) is said to form a <u>characteristic strip</u>, or <u>bicharacteristic</u>. However, in view of the role of these equations in geometrical optics and acoustics, we will refer to the curve $x_i(t)$ as a <u>ray</u> and equations (3.3) as the <u>ray equations</u>.

One noteworthy feature of (3.3) is the observation, due to the positive definite character of K_{ij}, that ψ is a monotonic non-increasing function of time along each ray.

Given a system of initial conditions, depending on a set of N-parameters (say $\gamma_1, \gamma_2, \ldots, \gamma_N$), then the solution $x_i(t; \gamma_k)$, $\psi(t; \gamma_k)$ of (3.3) provide an N+1 parameter parametric solution of (2.8), so long as the Jacobian

$$J(t; \gamma_k) = \frac{\partial(x_1, x_2, \ldots, x_N)}{\partial(\gamma_1, \gamma_2, \ldots, \gamma_N)} \tag{3.4}$$

does not vanish identically.

Having a solution of (2.8), we may proceed to the solution of the transport equations (2.10).

By (3.3), along each ray we have

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \frac{dx_i}{dt}\frac{\partial}{\partial x_i} = \frac{\partial}{\partial t} + \left(u_i - 2K_{ij}\frac{\partial \psi}{\partial x_j}\right)\frac{\partial}{\partial x_i}$$

whence (2.10) becomes

$$\frac{dA^{(0)}}{dt} = A^{(0)}\left[\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial \psi}{\partial x_j}\right) - \frac{\partial u_i}{\partial x_i}\right] \tag{3.5a}$$

$$\frac{dA^{(n)}}{dt} = A^{(n)}\left[\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial \psi}{\partial x_j}\right) - \frac{\partial u_i}{\partial x_i}\right] + \frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial A^{(n-1)}}{\partial x_j}\right) \tag{3.5b}$$

That is, the transport equations are reduced to an iterative system of ordinary differential equations along these rays.

A straightforward integration of (3.5a) and (3.5b) is possible, but it is easier and faster to proceed as follows:

It can be shown that the Jacobian (3.4) satisfies the following equation along the rays:

$$\frac{dJ}{dt} = J\left(\frac{\partial}{\partial x_i}\frac{dx_i}{dt}\right) \tag{3.6}$$

On substituting from (3.3), we have

$$\frac{dJ}{dt} = J\left[\frac{\partial u_i}{\partial x_i} - 2\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial \psi}{\partial x_j}\right)\right]$$

or, with (3.5a)

$$\frac{d}{dt}\left(A^{(0)}J^{1/2}\right) = -\frac{1}{2}A^{(0)}J^{1/2}\frac{\partial u_i}{\partial x_i} \tag{3.7}$$

In the event that the given flow is non-divergent $\left(\frac{\partial u_i}{\partial x_i} = 0\right)$ then $A^{(0)}J^{1/2}$ is constant on each ray, or

$$A^{(0)} = f(\gamma_1, \gamma_2, \ldots, \gamma_N)\left[J(t; \gamma_1, \gamma_2, \ldots, \gamma_N)\right]$$

where $f(\gamma_1, \gamma_2, \ldots, \gamma_N)$ is an arbitrary function of the ray parameters only.

If the flow is divergent, on the other hand, we fin$_\wedge$

$$A^{(0)} = f(\gamma_1, \gamma_2, \ldots, \gamma_N)\left[J(t; \gamma_1, \gamma_2, \ldots, \gamma_N)\right]^{-1/2} \exp\left(-\tfrac{1}{2}\int_{t_0}^{t}\frac{\partial u_i}{\partial x_i}d\tau\right) \tag{3.8}$$

the integration being carried out along the ray.

If initial conditions are given for $A^{(0)}$ at time t_o and $J(t_0; \gamma_1, \gamma_2, \ldots, \gamma_N) \neq 0$, then

$$A^{(0)}(t) = A^{(0)}(t_0)\left[\frac{J(t_0)}{J(t)}\exp\left(-\int_{t_0}^{t}\frac{\partial u_i}{\partial x_i}d\tau\right)\right]^{1/2} \tag{3.9}$$

where the dependence on the parameters is understood.

With a solution $A^{(0)}(t; \gamma_1, \gamma_2, \ldots, \gamma_N)$ to (3.5a), we may solve (3.5b) by setting

$A^{(n)}(t) = F_n(t)A^{(0)}(t)$, or using (3.5a) and (3.5b)

$$A^{(0)}\frac{dF_n}{dt} = \frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial}{\partial x_j}\left(A^{(0)}F_{n-1}\right)\right)$$

whence

$$A^{(n)}(t) = A^{(n)}(t_0) + A^{(0)}(t)\int_{t_0}^{t}\left[A^{(0)}(\tau)\right]^{-1}\left(\frac{\partial}{\partial x_i}K_{ij}\left(\frac{\partial}{\partial x_j}A^{(n-1)}\right)\right)d\tau \tag{3.10}$$

yields a constructive, iterative procedure to obtain the remaining transport terms.

A geometrical interpretation of (3.8) that is frequently illuminating is as follows: A ray tube is a region of space-time generated by rays (see fig. 1). If the ray tube is sufficiently thin, the Jacobian J is proportional to the volume (or hypervolume) of the intersection of the tube with hyperplanes t= const.

By (3.8), the quantity

$$Q = (A^{(0)})^2 \exp\left[\int_{t_0}^{t} \frac{\partial u_i}{\partial x_i} d\tau \right] \tag{3.11}$$

is inversely proportional to the Jacobian.

Accordingly, for sufficiently thin ray tubes with cross-sectional volume $d\,\sigma(t)$,

$$Q(t)d\,\sigma(t) = \text{const.} \tag{3.12}$$

That is, Q (t), given by (3.11), represents the density of some quantity that is being transported conservatively with the rays, i.e. (3.8) represents a conservation law.

In the theories of optics and acoustics, the corresponding quantity is the square of the wave amplitude, which measures the energy density transported by the wave. This suggests that $Q(t)$ may also be connected with some physically significant quantity.

In any event, (3.11), (3.12) offer a means of obtaining geometrically the transport $A^{(0)}$ when the rays, and hence the cross sectional areas, are found. This procedure is especially simple for non-divergent flows.

4. Initial Conditions

As with other Hamilton systems, the solutions to (3.3) are fully specified, given initial values for the x_i, ν, p_i for each ray of the N-parameter family. We are now faced with the problem of obtaining such conditions, corresponding to the given initial conditions for (2.5).

Historically, this problem has been attacked heuristically (Lewis, 1964), (Cohen and Lewis, 1967), (Lewis and Keller, 1963), usually from "physical intuition", or by comparison with a known solution to a simpler "cononical problem" which preserves significant features of the given problem. In some cases (Lewis and Keller, 1963), boundary layer methods offer a more direct means of obtaining boundary conditions. The complexity of the latter methods, however, leads us to use the former approach here.

In the case of the instantaneous point source problem, the total concentration of diffusant is located initially at the origin. It seems plausible, then, to assume that the rays themselves emanante from the origin. By this reasoning, for every ray in our family, we should assume $x_i(0) = 0$.

In order to have a parametric representation in a space-time neighborhood of the origin, a ray must pass through every point. In order for this to happen, we must allow the initial values for $\frac{d}{d\tau} x_i$ to take on all possible sets of values, one set for each ray. By (3.3), this implies that the initial values for Pi, take on all finite sets of values, one set for each ray. Conversely, a given set of initial values p_i^0 will determine each ray. Hence we may use p_i^0, rather than γ_i, to parametrize our family of rays.

Thus, the boundary conditions for our problem are

$$\left.\begin{aligned} x_i(0) &= 0 \\ p_i(0) &= p_i^0 \\ \psi(0) &= \psi^0(p_i^0) \end{aligned}\right\} \qquad (4.1)$$

But, if $\psi(x_i,t)$, defined parametrically by (3.3) and (4.1), is to satisfy

$$p_i = \frac{\partial \psi}{\partial x_i}$$

and the Jacobian $\frac{\partial(x_1, x_2, \ldots, x_N)}{\partial(p_1^0, p_2^0, \ldots, p_N^0)}$ does not vanish identically, it can be shown that $\frac{\partial \psi^0}{\partial p_i^0} = 0$; i.e. the initial value ψ^0 is constant for the entire family of rays.

Our boundary conditions for the point source problem now consists of

$$\begin{aligned} x_i(0) &= 0 \\ p_i(0) &= p_i^0 \\ \psi(0) &= \psi^0 \end{aligned} \qquad (4.2)$$

where the p_i^0 take on the entire range of values $-\infty < p_i^0 < \infty$, and the ψ^0 is fixed.

The range of values for the p_i^0 is unrestricted owing to the parabolic character of (2.5). For hyperbolic equations, the p_i^0 must be restricted so that all rays remain inside the characteristic conoid,

and for non-dispersive hyperbolic equations, such as the wave equation, the rays must lie on the conoid itself (see Lewis, 1964).

To complete the analysis of initial conditions, we need a value for ψ^0, a condition on the behavior of the transport terms $A^{(n)}$ near t = 0, and a value for the α in the expansion (2.7b).

To obtain these, we consider the following "canonical problem": $u_i \equiv 0$, K_{ij} = const. This is the classical heat conduction problem, the solution of which has been frequently published (Carslaw and Jaeger, 1947), (Lewis, 1966), (Courant and Hilbert, 1962) and many others.

The ray equations become

$$\left.\begin{aligned} \frac{dx_i}{dt} &= -2K_{ij}p_j \\ \frac{d\psi}{dt} &= -K_{ij}p_ip_j \\ \frac{dp_i}{dt} &= 0 \end{aligned}\right\} \qquad (4.3)$$

and the boundary conditions

$$\begin{aligned} x_i(0) &= 0 \\ p_i(0) &= p_i^0 \\ \psi(0) &= \psi^0 \end{aligned}$$

whence

$$\begin{aligned} p_i &= p_i^0 = \text{const.} \\ x_i &= -2K_{ij}p_j^0 t \\ \psi &= \psi^0 - K_{ij}p_i^0 p_j^0 t \end{aligned}$$

We then have $-2t\rho_j^\circ = (K^{-1})_{ij}\, x_i.$

(where $(K^{-1})_{ij}$ is defined such that $(K^{-1})_{ij} K_{jk} = \delta_{ik}$, δ_{ik} being the Kronecker delta) and so

$$\psi = \psi_\circ^\circ - \frac{1}{4t}(K^{-1})_{ij}\, x_i x_j \tag{4.4}$$

The behavior of the first transport term $A^{(0)}(x_i,t)$ is determined by the Jacobian

$$J = \frac{\partial(x_i)}{\partial(\rho_j^\circ)} = (-2t)^N \det[K_{ij}]$$

from which

$$A^{(0)}(t) \propto |J|^{-1/2} = \frac{1}{(2t)^{N/2}\{\det[K_{ij}]\}^{1/2}}$$

Thus, $A^{(0)}(t)$ is proportional to $t^{-N/2}$ on each ray, where N is the number of dimensions. This may also be seen as follows: The rays are all straight lines through the origin $x_i = 0,\ t = 0$, hence the ray tubes are all cones through the origin (see fig. 2). The t = const. sections of a given cone have linear dimensions directly proportional to t, so the N-dimensional volume of these sections, and hence the Jacobian, is proportional to t^N. By (3.11), (3.12)

$$(A^{(0)})^2 \propto \frac{1}{t^N} \qquad A^{(0)} \propto \frac{1}{t^{N/2}}$$

Since $A^{(0)}(t)$ necessarily is singular at t = 0, the initial condition on $A^{(0)}$ must define, not $A^{(0)}(0)$, but the proportionality factor relating $A^{(0)}(t)$ and $t^{-N/2}$. This factor may differ for

different rays, so we have

$$A^{(0)}(x_i,t) = t^{-N/2}\,\phi^*(\rho_k^\circ) = t^{-N/2}\,\phi\left(\frac{x_i}{t}\right)$$

where ϕ^*, and ϕ are arbitrary functions.

Hence, the ray method obtains a first order approximation to C in the form:

$$C^{(0)}(x_i,t) = \lambda^\alpha t^{-N/2}\,\phi\left(\frac{x_i}{t}\right) e^{\lambda\psi^\circ} e^{-\frac{\lambda}{4t}(K^{-1})_{ij} x_i x_j} \tag{4.5}$$

with α, ψ° constants and ϕ a function yet to be determined.

The actual solution is

$$C = \left(\frac{\lambda}{4\pi t}\right)^{N/2}\{\det[K_{ij}]\}^{-1/2}\, e^{-\frac{\lambda}{4t}(K^{-1})_{ij} x_i x_j} \tag{4.6}$$

corresponding to $\alpha = N/2$, $\phi = (4\pi)^{-N/2}\{\det[K_{ij}]\}^{-1/2}$ and $\psi^\circ = 0$

Actually, $C^{(0)}$ as given in (4.5) satisfies (2.5) whenever $\phi(\xi_i)$ satisfies

$$\frac{\partial}{\partial\xi_i} K_{ij} \frac{\partial\phi}{\partial\xi_j} = 0 \tag{4.7}$$

Solutions of (4.7) are given by $\phi(\xi_i) = \varphi((K^{-1})_{ij}\xi_j)$ where φ is any harmonic function (solution of Laplace's equation in N variables).

Moreover, if the φ is exponentially bounded as $|\eta_i| = |(K^{-1})_{ij}\xi_j| \to \infty$ then, for all t

$$\int C^{(0)}(x_i,t)\,dx_i = (4\pi)^{N/2}\,\phi(0)\,\lambda^{\alpha-N/2}\, e^{\lambda\psi^\circ}\{\det[K_{ij}]\}^{1/2}$$

so the total concentration is unity, independent of λ , provided

$$\phi(0) = (4\pi)^{-N/2} \{ det [K_{ij}] \}^{-1/2}, \quad \alpha = N/2, \quad \psi^{\circ} = 0 \tag{4.8}$$

Since $\lim_{t \downarrow 0} C^{(0)}(x_i,t) = 0$ when $x_i x_i \neq 0$ and $\int C^{\circ}(x_i,t)\, d x_i = 1$ and there are an infinite number of exponentially bounded harmonic functions with a given value at the origin, it appears that there are an infinite number of solutions to our problem.

However, it can be shown that $C^{0}(x_i,t)$ tends to the Dirac delta function only when ϕ is a constant. For all other solutions, $C^{0}(x_i,t)$ tends to a linear combination of the Dirac delta function with its derivatives.

Since the K_{ij} are assumed positive definite and symmetric, we may, without loss of generality assume the coordinates x_i chosen so K_{ij} is diagonal, i. e.

$$K_{ij} = \begin{cases} K_i > 0 & if \ i = j \\ 0 & if \ i \neq j \end{cases}$$

In this case, the solution (4.6) reduces to the standard forms

$$C = \left(\frac{\lambda}{4\pi t}\right)^{N/2} \frac{1}{(K_1 K_2 \cdots K_N)^{1/2}} \exp\left\{ -\frac{\lambda}{4t}\left[\frac{x_1^2}{K_1} + \frac{x_2^2}{K_2} + \cdots + \frac{x_N^2}{K_N} \right]\right\}$$

if the K_i differ, or

$$C = \left(\frac{\lambda}{4\pi K t}\right)^{N/2} \exp\left\{ -\frac{\lambda\, x_i x_i}{4Kt} \right\}$$

if the K_i are all equal to a constant K.

On the basis of comparison with the canonical problem, we will assume, for other instantaneous point source problems, that the

corresponding initial values for the ray equations will be

$$\begin{aligned} x_i(0) &= 0 \\ p_i(0) &= p_i^{\circ} \\ \psi(0) &= 0 \end{aligned} \tag{4.9}$$

where the p_i° take on all values and, for the first transport term,

$$A^{(0)}(t) \approx \left(\frac{1}{4\pi t}\right)^{N/2} \frac{1}{\{ det [K_{ij}^{\circ}] \}^{1/2}} \quad as \ t \downarrow 0 \tag{4.10}$$

where $K_{ij}^{\circ} = K_{ij}(x_i(0), 0)$ is the value of K_{ij} at the origin at time zero. Furthermore, the expansion (2.7) will be in the form

$$C(x_i,t) = \exp\{\lambda \psi(x_i,t)\} \sum_{n=0}^{\infty} \lambda^{N/2 - n} A^{(n)}(x_i,t)$$

i.e. $\alpha = N/2$.

The initial conditions for the higher order transport terms are still unspecified. The present "canonical problem", offers no assistance in obtaining these conditions, since the exact solution is precisely the truncated asymptotic expansion. Nonetheless, the last problem treated in the following section will illustrate how these conditions may be obtained from two principles: First, that $A^{(n)}/A^{(0)}$ can be continuously extended to t = o, secondly, that no transport term $A^{(n)}$, for $n > 0$, contributes to the strength of the source.

5. Examples

A. Linear Shear Flow in two Dimensions

Write $u = u_1$, $v = u_2$, $K_x = K_{11}$, $K_y = K_{22}$; $x = x_1$ and $y = x_2$.

Suppose $u = by$, $v = 0$ and $K_{12} = 0$; K_x, K_y and b are constants.

Then equation (2.5) becomes

$$\frac{\partial c}{\partial t} + by\frac{\partial c}{\partial x} = \frac{1}{\lambda} K_x \frac{\partial^2 c}{\partial x^2} + \frac{1}{\lambda} K_y \frac{\partial^2 c}{\partial y^2} \tag{5.1}$$

corresponding to diffusion from a point source in a parallel two dimensional flow field of linear shear (see fig. 3).

The ray equations (3.3) become

$$\left.\begin{aligned} \frac{dx}{dt} &= by - 2K_x p \\ \frac{dy}{dt} &= -2K_y q \\ \frac{d\psi}{dt} &= -K_x p^2 - K_y q^2 \\ \frac{dp}{dt} &= 0 \\ \frac{dq}{dt} &= -bp \end{aligned}\right\} \tag{5.2}$$

when we set $p = p_1$, $q = p_2$

The boundary conditions are

$$\left.\begin{aligned} x(0) = y(0) = \psi(0) = 0 \\ p(0) = p^\circ, \quad q(0) = q^\circ \end{aligned}\right\} \tag{5.3}$$

and the solution is easily found to be

$$\left.\begin{aligned} & p = p^\circ = \text{const.} \qquad q = -bp^\circ t + q^\circ \\ & y = K_y b p^\circ t^2 - 2K_y q^\circ t \\ & x = p^\circ\left(\tfrac{1}{3} K_y b^2 t^3 - 2K_x t\right) - K_y b q^\circ t^2 \\ & \psi = -(p^\circ)^2\left[K_x t + \tfrac{1}{3} K_y b^2 t^3\right] + p^\circ q^\circ K_y b t^2 - (q^\circ)^2 K_y t \end{aligned}\right\} \tag{5.4}$$

Now, x and y are linear functions of p° and q°, with coefficients depending on the time, while ψ is a quadratic form in p° and q°. On eliminating p° and q° by writing them as linear functions of x and y, we find

$$\psi = \frac{1}{4t(1+\tau^2/12)}\left[-\frac{x^2}{K_x} + \frac{xy\tau}{\ell} - \frac{y^2}{K_y}\left(1+\frac{\tau^2}{3}\right)\right] \tag{5.5}$$

where $\tau = b\left(\dfrac{K_y}{K_x}\right)^{1/2} t$, $\quad \ell = (K_x K_y)^{1/2}$

The transport terms are found through the Jacobian

$$J = \frac{\partial(x,y)}{\partial(p^\circ, q^\circ)} = 4K_x K_y \tau^2\left(1 + \frac{1}{12}\tau^2\right).$$

and the first transport term is, by (3.8), (4.10)

$$A^{(0)} = \frac{1}{(4\pi K_x K_y)^{1/2}} \frac{1}{t} \frac{1}{(1+\tau^2/12)^{1/2}}$$

which is independent of x and y.

Our solution for uni-directional shear flow in two dimensions, then is

$$C^\circ = \frac{\lambda}{4\pi t(1+\tau^2/12)^{1/2}} \cdot \frac{1}{\ell} \cdot \exp\left\{\frac{-\lambda}{4t(1+\tau^2/12)}\left[\frac{x^2}{K_x} - \frac{xy\tau}{\ell} + \frac{y^2}{K_y}(1+\tau^2/3)\right]\right\} \tag{5.6}$$

The result (5.6) agrees with that of (Neuringer, 1967) and (Okuba, 1968). It should be noted that the solution approaches the classical solution (4.6) for no shear motion when $\tau << 1$; accordingly, it is reasonable to define τ as the time scale for effects due to the shear, while t represents the time scale for diffusion effects.

The level curves of (5.6), like the level curves for the classical solution, are co-axial ellipses centered at the origin. Unlike the classical solution, the axes are not stationary with time, but rotate under the influence of the shear. Surprisingly, the amount of this rotation need not be equal to the rotation of the underlying fluid, nor even in the same direction. Its magnitude and direction depend on the relative values of K_x, K_y and b.

B. Flows Depending Linearly on the Coordinates

In the case of linear shear in two dimensions, the asymptotic expansion obtained by the ray method truncated to one term, and thus became the exact solution. This fortuitous circumstance also occurs whenever the diffusion coefficients K_{ij} are independent of, and the flow velocities u_i are linearly depended on, the coordinates x_i.

Specifically, we suppose

$$\left.\begin{aligned} K_{ij} &= K_{ij}(t) \\ u_i(x_i,t) &= u_i^{\circ}(t) + \omega_{ij}(t)\,x_j \end{aligned}\right\} \qquad (5.7)$$

where the $K_{ij}(t)$, $u_i^{\circ}(t)$ and $\omega_{ij}(t)$ are arbitrary continuous functions of time.

In this case, our ray equations (3.3) are more conveniently written in the matrix form

$$\begin{aligned} \frac{dX}{dt} &= U + \Omega X - 2KP \\ \frac{d\nu}{dt} &= -P^T K P \\ \frac{dP}{dt} &= -\Omega^T P \end{aligned} \qquad (5.8)$$

where X, U and P are column vectors and Ω and K matrices with components $x_i, u_i^{\circ}, p_i, \omega_{ij}$ and K_{ij}, respectively. The superscript T denotes transpose.

The problem of solving (5.8) reduces to that of solving the homogeneous equation:

$$\frac{dP}{dt} = -\Omega^T P \qquad (5.9)$$

Indeed, let $M(t)$ denote a fundamental solution (a non-singular matrix-valued solution) of (5.9). Then $[M^{-1}]^T(t)$ is a solution of the homogeneous equation

$$\frac{dX}{dt} = \Omega X$$

In consequence the non-homogeneous equation for in (5.8) becomes

$$\frac{d}{dt}[M^T X] = M^T U - 2M^T P$$

The solution for P is in the form

$$P = M(t)\Gamma$$

where Γ is an arbitrary constant column vector, whose coefficients γ_i represent the ray parameters.

Then

$$X = [M^T]^{-1}\left\{\int_0^t [M^T U - 2M^T K P]\,d\tau\right\}$$

or

$$X = [M^T]^{-1}\int_0^t M^T U\,d\tau - 2[M^T]^{-1}\left\{\int_0^t M^T K M\,d\tau\right\}\Gamma \qquad (5.10)$$

while

$$\psi = -\Gamma^T \int_0^t M^T K M\,d\tau\,\Gamma \qquad (5.11)$$

We denote the matrix $\int_0^t M^T K M\,d\tau$ by S and note that S is a positive definite symmetric matrix except when t=0, in which case S vanishes.

Consequently, for $t > 0$, Γ, and hence ψ may be found in terms of X and t:

$$\Gamma = -\tfrac{1}{2} S^{-1}\left\{M^T X - \int_0^t M^T U\,d\tau\right\}$$

$$\psi = -\tfrac{1}{4}\left[M^T X - \int_0^t M^T U\,d\tau\right]^T [S^{-1}]^T S\, S^{-1}\left[M^T X - \int_0^t M^T U\,d\tau\right]$$

or

$$\psi = -\tfrac{1}{4}\left[M^T X - \int_0^t M^T U\,d\tau\right]^T S^{-1}\left[M^T X - \int_0^t M^T U\,d\tau\right] \qquad (5.12)$$

The first transport term $A^{(o)}$ is obtained from

$$J(t) = \det\left[\frac{\partial x_i}{\partial \beta_j}\right] = \det\left[2[M^T]^{-1} S\right]$$

We note that, as $t \to 0$

$$J(t) \sim 2^N \det K(0) \det M(0)\, t^N$$

whence, by (3.8 and (4.10),

$$A^{(0)} = \frac{1}{(\pi)^{N/2}}\left[\frac{\det M(0)}{J(t)}\right]^{1/2} \exp\left\{\tfrac{1}{2}\int_0^t \frac{\partial u_i}{\partial x_i}\,d\tau\right\}$$

Since $A^{(o)}$ is independent of X, we need no other transport terms.

The divergence $\frac{\partial u_i}{\partial x_i}$ of the flow is given by $Tr[\Omega] = Trace[\Omega]$ so the complete solution of

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i}(u_i C) = \frac{1}{\lambda}\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial c}{\partial x_j}\right)$$

for instantaneous point source diffusion in the case $K_{ij} = K_{ij}(t)$

$u_i = u_i^o(t) + \omega_{ij}(t)\, x_j$

is given by

$$C = \lambda^{N/2} A^{(0)} \exp\{-\lambda\psi(x,t)\} \exp\left\{-\tfrac{1}{2}\int_0^t Tr[\Omega]\,d\tau\right\} \qquad (5.13)$$

where

$$\left.\begin{aligned} A^{(0)} &= \frac{1}{(4\pi)^{N/2}}\left[\frac{\det M(0)\det M(t)}{\det S(t)}\right]^{1/2} \\ \psi(x,t) &= -\tfrac{1}{4}\left[M^T X - \int_0^t M^T U\,d\tau\right]^T S^{-1}\left[M^T X - \int_0^t M^T U\,d\tau\right] \\ S(t) &= \int_0^t M^T K M\,d\tau \end{aligned}\right\} \qquad (5.14)$$

and $M(t)$ is any fundamental solution of

$$\frac{d}{dt} M = -\Omega^T M$$

<u>Case 1</u> Suppose N=2 and

$$U = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad \Omega = \begin{bmatrix} 0 & b \\ 0 & 0 \end{bmatrix}, \quad K = \begin{bmatrix} K_x & 0 \\ 0 & K_y \end{bmatrix}$$

where K_x, K_y, b are constants. This is simply example A, of linear shear flow in two dimensions.

Then

$$M = \begin{bmatrix} 1 & 0 \\ -bt & 1 \end{bmatrix} \qquad Tr\,[\Omega] = 0$$

$$S = \begin{bmatrix} K_x t + \frac{1}{3} b^2 t^3 K_y & -\frac{1}{2} K_y b t^2 \\ -\frac{1}{2} K_y b t^2 & K_y t \end{bmatrix}$$

$$S^{-1} = \frac{1}{K_x K_y t^2 + \frac{1}{12} b^2 t^4 K_y^2} \begin{bmatrix} K_y t & \frac{1}{2} K_y b t^2 \\ \frac{1}{2} K_y b t^2 & K_x t + \frac{1}{3} b^2 t^3 K_y \end{bmatrix}$$

$$\Psi = -\frac{1}{4} X^T [M S^{-1} M^T] X = \frac{1}{4 K_y K_x t^2 \left(1 + \frac{1}{12} \frac{K_y}{K_x} b^2 t^2\right)} [x, y] \begin{bmatrix} K_y t & -\frac{1}{2} K_y b t^2 \\ -\frac{1}{2} K_y b t^2 & K_x t + \frac{1}{3} b^2 t^3 K_y \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

and

$$A^{(0)} = \frac{1}{4\pi} \frac{1}{(K_x K_y)^{1/2} t} \frac{1}{\left(1 + \frac{1}{12} \frac{K_y}{K_x} b^2 t^2\right)^{1/2}}$$

Thus, C, as given by (5.13) results in precisely (5.6)

Case 2. Linear Shear in Three Dimensions.

In this case, we have

$$U = \begin{bmatrix} U_0(t) \\ 0 \\ 0 \end{bmatrix} \qquad \Omega = \begin{bmatrix} 0 & \omega_y & \omega_z \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad K = \begin{bmatrix} K_x & 0 & 0 \\ 0 & K_y & 0 \\ 0 & 0 & K_z \end{bmatrix}$$

(c.f.(Okuba, 1968)) where $\omega_y, \omega_z, K_x, K_y, K_z$ are constants.

Then

$$M(t) = \begin{bmatrix} 1 & 0 & 0 \\ -\omega_y t & 1 & 0 \\ -\omega_z t & 0 & 1 \end{bmatrix}$$

$$S(t) = \begin{bmatrix} K_x t + \frac{1}{3} \phi t^3 & -\frac{1}{2} K_y \omega_y t^2 & -\frac{1}{2} K_z \omega_z t^2 \\ -\frac{1}{2} K_y \omega_y t^2 & K_y t & 0 \\ -\frac{1}{2} K_z \omega_z t^2 & 0 & K_z t \end{bmatrix}$$

where $\phi = K_y \omega_y^2 + K_z \omega_z^2$.

$$\det S(t) = K_x K_y K_z t^3 \left[1 + \frac{1}{12} \tau^2 \right]$$

where $\tau = t \left[\frac{\phi}{K_x}\right]^{1/2}$.

$$S(t)^{-1} = \frac{1}{\left(1 + \frac{1}{12} \tau^2\right)} \begin{bmatrix} \frac{1}{K_x t} & \frac{\omega_y}{2 K_x} & \frac{\omega_z}{2 K_x} \\ \frac{\omega_y}{2 K_x} & \frac{1}{K_y t} + \frac{\omega_y^2 t}{3 K_x} + \frac{K_z \omega_z^2 t}{12 K_x K_y} & \frac{\omega_y \omega_z t}{4 K_x} \\ \frac{\omega_z}{2 K_x} & \frac{\omega_y \omega_z t}{4 K_x} & \frac{1}{K_z t} + \frac{\omega_z^2 t}{3 K_x} \end{bmatrix}$$

$$\Psi = -\frac{1}{4} [x^*, y, z] \left[S(t)^{-1} \right] \begin{bmatrix} x^* \\ y \\ z \end{bmatrix}$$

where $x^* = x - \int_0^t U_0(t')\,dt' + \omega_y y t + \omega_z z t$

Some further algebraic manipulation leads to

$$\Psi = -\frac{1}{4\left(1 + \frac{1}{12}\tau^2\right)} \left\{ \frac{\left[x - \int_0^t U(t')dt'\right]^2}{K_x t} + \frac{y^2}{K_y t}\left[1 + \frac{\tau_y^2}{3} + \frac{\tau_z^2}{12}\right] + \frac{z^2}{K_z t}\left[1 + \frac{\tau_z^2}{3} + \frac{\tau_y^2}{12}\right] + \left[x - \int_0^t U(t')dt'\right] \frac{\omega_y y + \omega_z z}{K_x} + \frac{1}{2} \frac{\omega_y \omega_z t y z}{K_x} \right\} \tag{5.15}$$

where $\tau_y = \omega_y t \left[\frac{K_y}{K_x}\right]^{1/2}$, $\tau_z = \omega_z t \left[\frac{K_z}{K_x}\right]^{1/2}$, $\tau^2 = \tau_y^2 + \tau_z^2$

Moreover

$$A^{(0)}(t) = \frac{1}{(4\pi)^{3/2}} \frac{1}{[\det S]^{1/2}} = \frac{1}{(4\pi t)^{3/2}} \cdot \frac{1}{(K_x K_y K_z)^{1/2}} \cdot \frac{1}{[1+\tau^2/12]^{1/2}} \quad (5.16)$$

with these expressions for $A^{(0)}, \psi$, the solution is

$$C^{(0)}(x,y,z,t) = \lambda^{3/2} A^{(0)}(t) \quad \exp\{-\lambda\psi\} \quad (5.17)$$

For $\lambda = 1$, this corresponds exactly to equation (3) of (Okuba, 1968)

Case 3. Bilinear Shear in Two Dimensions

We now consider diffusion in a flow which is not parallel, and, for simplicity, we restrict ourselves again to two dimensions. We consider the case where $u = \omega_1 y$, $v = \omega_2 x$ and, for simplicity $u^0 = v^0 = K_{12} = K_{21} = 0$ and ω_1, ω_2, K_x and K_y are constants.

Thus

$$\Omega = \begin{bmatrix} 0 & \omega_1 \\ \omega_2 & 0 \end{bmatrix} \qquad K = \begin{bmatrix} K_x & 0 \\ 0 & K_y \end{bmatrix}$$

and (2.5) is

$$\frac{\partial c}{\partial t} + \omega_1 y \frac{\partial c}{\partial x} + \omega_2 x \frac{\partial c}{\partial y} = \frac{1}{\lambda}\left(K_x \frac{\partial^2 c}{\partial x^2} + K_y \frac{\partial^2 c}{\partial y^2}\right)$$

The eigenvalues of Ω are $\pm(\omega_1\omega_2)^{1/2}$, and we have qualitatively different flow patterns according as $\omega_1\omega_2 > 0$ or $\omega_1\omega_2 < 0$.

If $\omega_1\omega_2 > 0$, the streamlines are open curves in the form of co-asymptotic hyperbolas, while if $\omega_1\omega_2 < 0$, they take on the form of co-axial ellipses (see Figs. 4 and 5).

/s /and 5

We shall carry out the computations for the first case only, i.e. that of $\omega_1\omega_2 > 0$. Let $\mu = (\omega_1\omega_2)^{1/2}$. Then

$$M(t) = \begin{bmatrix} \mu e^{\mu t} & \omega_2 e^{-\mu t} \\ -\omega_1 e^{\mu t} & \mu e^{-\mu t} \end{bmatrix}$$

is a fundamental solution for

$$\frac{d}{dt} M = -\Omega^T M.$$

Then

$$S(t) = \frac{(K_x\omega_2 + K_y\omega_1)\sinh(\mu t)}{\mu} \begin{bmatrix} \omega_1 e^{\mu t} & 0 \\ 0 & \omega_2 e^{-\mu t} \end{bmatrix} + (K_x\omega_2 - K_y\omega_1) \begin{bmatrix} 0 & \mu t \\ \mu t & 0 \end{bmatrix}$$

$$\det S(t) = (K_x\omega_2 + K_y\omega_1)^2 \sinh^2 \mu t - (K_x\omega_2 - K_y\omega_1)^2 \mu^2 t^2$$

$$S(t)^{-1} = \frac{1}{\Delta}\left\{ \frac{(K_x\omega_2 + K_y\omega_1)\sinh \mu t}{\mu} \begin{bmatrix} \omega_2 e^{-\mu t} & 0 \\ 0 & \omega_1 e^{\mu t} \end{bmatrix} + (K_x\omega_2 - K_y\omega_1) \begin{bmatrix} 0 & -\mu t \\ -\mu t & 0 \end{bmatrix} \right\}$$

where

$$\Delta = \det S(t).$$

$$M S^{-1} M^T = \frac{2\mu}{\Delta} \left\{ (K_x\omega_2 + K_y\omega_1) \begin{bmatrix} \omega_2 \cosh \mu t & -\mu \sinh \mu t \\ -\mu \sinh \mu t & \omega_1 \cosh \mu t \end{bmatrix} + (K_x\omega_2 - K_y\omega_1)\mu t \begin{bmatrix} -\omega_2 & 0 \\ 0 & \omega_1 \end{bmatrix} \right\}$$

and

$$\psi = -\tfrac{1}{4}[x, y] M S^{-1} M^{T} \begin{bmatrix} x \\ y \end{bmatrix} = f_{11}(t)\, x^2 + 2 f_{12}(t)\, xy + f_{22}(t)\, y^2 \qquad (5.18)$$

where

$$\left.\begin{aligned} f_{11}(t) &= -\frac{\mu \omega_1}{2\Delta} \left\{ (K_x \omega_2 + K_y \omega_1) \sinh \mu t \cosh \mu t - (K_x \omega_2 - K_y \omega_1) \mu t \right\} \\ f_{12}(t) &= \frac{\mu^2}{2\Delta} (K_x \omega_2 + K_y \omega_1) \sinh^2 \mu t \\ f_{22}(t) &= -\frac{\mu \omega_1}{2\Delta} \left\{ (K_x \omega_2 + K_y \omega_1) \sinh \mu t \cosh \mu t + (K_x \omega_2 - K_y \omega_1) \mu t \right\} \end{aligned}\right\} \qquad (5.19)$$

$$\Delta = (K_x \omega_2 + K_y \omega_1)^2 \sinh^2 \mu t - (K_x \omega_2 - K_y \omega_1)^2 \mu^2 t^2 \qquad (5.20)$$

The transport term is

$$A^{(0)} = \frac{1}{4\pi} \left[\frac{\det M(0) \det M(t)}{\det S} \right]^{1/2}$$

or

$$A^{(0)} = \frac{1}{4\pi} \frac{2\mu^2}{\Delta^{1/2}} \qquad (5.21)$$

and

$$C^{(0)} = \frac{\mu^2 \lambda}{2\pi \Delta^{1/2}} \exp\left\{ \lambda [f_{11}(t)\, x^2 + 2 f_{12}(t)\, xy + f_{22}(t)\, y^2] \right\}$$

If $\omega \omega_2 < 0$, we could write $(\omega_1 \omega_2)^{1/2} = \mu = i\tilde{\omega}$

Then a fundamental solution matrix is

$$M(t) = \begin{bmatrix} \tilde{\omega} \cos \tilde{\omega} t & -\omega_2 \sin \tilde{\omega} t \\ -\omega_1 \sin \tilde{\omega} t & \tilde{\omega} \cos \tilde{\omega} t \end{bmatrix}$$

We could use this matrix to obtain ψ, $A^{(0)}$, and $C^{(0)}$ as above, but it is simpler just to substitute $i\tilde{\omega}$ for μ in (5.18) through (5.21). If this is done, we find

$$C^{(0)}(x, y, t) = \lambda A^{(0)}(t) \exp[\lambda \psi(x, y, t)]$$

in which

$$\psi = f_{11}(t)\, x^2 + 2 f_{12}(t)\, xy + f_{22}(t)\, y^2 \qquad (5.22)$$

$$A^{(0)} = \frac{\tilde{\omega}^2}{2\pi \Delta^{1/2}} \qquad (5.23)$$

where

$$\left.\begin{aligned} f_{11}(t) &= -\frac{\tilde{\omega} \omega_2}{2\Delta} \left\{ (K_x \omega_2 - K_y \omega_1) \tilde{\omega} t - (K_x \omega_2 + K_y \omega_1) \sin \tilde{\omega} t \cos \tilde{\omega} t \right\} \\ f_{12}(t) &= \frac{\tilde{\omega}^2}{2\Delta} (K_x \omega_2 + K_y \omega_1) \sin^2 \tilde{\omega} t \\ f_{22}(t) &= -\frac{\tilde{\omega} \omega_1}{2\Delta} \left\{ (K_y \omega_1 - K_x \omega_2) \tilde{\omega} t - (K_x \omega_2 + K_y \omega_1) \sin \tilde{\omega} t \cos \tilde{\omega} t \right\} \end{aligned}\right\} \qquad (5.24)$$

and

$$\Delta = (K_x \omega_2 - K_y \omega_1)^2 \tilde{\omega}^2 t^2 - (K_x \omega_2 + K_y \omega_1)^2 \sin^2 \tilde{\omega} t \qquad (5.25)$$

As $t \downarrow 0$, in either case,

$$\left.\begin{aligned} f_{11}(t) &\approx -\frac{1}{4K_x t} + O(1) \\ f_{12}(t) &\approx O(1) \\ f_{22}(t) &\approx -\frac{1}{4K_y t} + O(1) \\ \text{and} \quad A^{(0)}(t) &\approx \frac{1}{4\pi(K_x K_y)^{1/2} t} + O(1) \end{aligned}\right\} \tag{5.26}$$

i.e.

$$C^{(0)}(x,y,t) \approx \frac{\lambda}{4\pi(K_x K_y)^{1/2} t}\, e^{-\frac{\lambda}{4t}\left(\frac{x^2}{K_x} + \frac{y^2}{K_y}\right)} \left(1 + O(t)\right) \tag{5.27}$$

as $t \downarrow 0$, so that these solutions both tend to the solution for classical diffusion in the absence of flow, and hence the behavior of $C^{(0)}$ is independent of streamline type for small t.

By contrast, as $t \to \infty$, the behavior of $C^{(0)}$ differs radically between the elliptic streamline case and the hyperbolic streamline case.

In the case $\omega_1\omega_2 < 0$ (elliptic streamlines),

$$\left.\begin{aligned} f_{11}(t) &\approx -\frac{\omega_2}{2(K_x\omega_2 - K_y\omega_1)t}\left(1 + O(t^{-1})\right) \\ f_{12}(t) &\approx O(t^{-2}) \\ f_{22}(t) &\approx -\frac{\omega_1}{2(K_y\omega_1 - K_x\omega_2)t}\left(1 + O(t^{-1})\right) \\ A^{(0)}(t) &\approx \frac{1}{2\pi}\left|\frac{\tilde{\omega}}{K_x\omega_2 - K_y\omega_1}\right| \frac{1}{t}\left(1 + O(t^{-1})\right) \end{aligned}\right\} \tag{5.28}$$

The level curves of ψ, and hence of $C^{(0)}$, for each value of t are co-axial ellipses. By (5.28) the axes of these ellipses tend to the coordinate axes (or rather, the principal axes of K_{ij}). Indeed, the behavior of $C^{(0)}$ for large time tends to the behavior of the classical solution for no flow, provided K_x and K_y are replaced by effective diffusion coefficients,

$$\begin{aligned} K_x^* &= \tfrac{1}{2}\left(K_x - \frac{\omega_1}{\omega_2} K_y\right) \\ K_y^* &= \tfrac{1}{2}\left(K_y - \frac{\omega_2}{\omega_1} K_x\right) \end{aligned} \tag{5.29}$$

respectively. In the event that $\omega_1 = -\omega_2$ (circular streamlines), the effective diffusion coefficients are both equal to the mean of K_x and K_y and we have effectively isotropic diffusion.

By contrast, when $\omega_1\omega_2 > 0$ (hyperbolic streamlines), the f_{ij} and $A^{(0)}$ tend to

$$\left.\begin{aligned} f_{11}(t) &\approx -\frac{\mu\,\omega_2}{2(K_x\omega_2 + K_y\omega_1)}\left(1 + O(t^2 e^{-2\mu t})\right) \\ f_{12}(t) &\approx \frac{\mu^2}{2(K_x\omega_2 + K_y\omega_1)}\left(1 + O(t^2 e^{-2\mu t})\right) \\ f_{22}(t) &\approx -\frac{\mu\,\omega_1}{2(K_x\omega_2 + K_y\omega_1)}\left(1 + O(t^2 e^{-2\mu t})\right) \\ A^{(0)}(t) &\approx \frac{\mu^2}{\pi|K_x\omega_2 + K_y\omega_1|}\, e^{-\mu t}\left(1 + O(t^2 e^{-2\mu t})\right) \end{aligned}\right\} \tag{5.30}$$

The transport term $A^{(0)}(t)$, which measures the maximum density at each time, tends exponentially to zero, rather than as $t^{-N/2}$, as in the classical solution and all other solutions to date.

Moreover, the level curves of ψ, and hence $C^{(0)}$ are ellipses, but the eccentricity of these ellipses increases with time until, as (5.30) implies, they degenerate into straight lines parallel to one of the asymptotes of the streamlines. This asymptote turns out to be the one in the downstream direction, (see fig. 4).

C. Variable Diffusion Coefficient

When the diffusion coefficients K_{ij} vary, or the velocities u_i vary nonlinearly, with the coordinates x_i, the computational complexity of the ray method increases. Computation of $\psi, A^{(0)}$ and x_i in terms of the ρ_i° and t remains straightforward, if tedious, but the inversion to obtain $\psi(x_i,t)$ and $A^{(0)}(x_i,t)$ becomes more difficult, as does the computation of the $A^{(n)}(x_i,t)$, $n>0$, which no longer can be expected to vanish. Fortunately, it often happens that the $A^{(0)}$ term is sufficient to obtain qualitative, and even quantitative, features of the solution.

These difficulties decrease when we revert to one dimensional problems. To illustrate the behavior of higher order transport terms, we consider the situation of one-dimensional diffusion with vanishing flow component, and a diffusion coefficient varying linearly with the coordinate.

Thus,

$$\frac{\partial c}{\partial t} = \frac{1}{\lambda}\frac{\partial}{\partial z} K \frac{\partial c}{\partial z} \qquad K = \alpha(z+z^*) \tag{5.31}$$

$\alpha>0$ and $z^*>0$ are constants.

In the domain of definition of the problem we must have $K>0$, since the problem is well posed only when K_{ij} is positive definite. Accordingly, we can no longer deal with infinite domains, but with the domain $z>-z^*$. This suggests a boundary condition will be required at $z=-z^*$. We will return to this point later.

The ray equations for diffusion from a point source at the origin are

$$\left.\begin{aligned} \frac{dz}{dt} &= -2K\rho \\ \frac{d\psi}{dt} &= -K\rho^2 \\ \frac{d\rho}{dt} &= \frac{\partial K}{\partial z}\rho^2 = \alpha\rho^2 \end{aligned}\right\} \tag{5.32}$$

with boundary conditions

$$z(0) = \psi(0) = 0 \qquad \rho(0) = \rho^{\circ} \tag{5.33}$$

and the solution is

$$\left.\begin{aligned} \rho &= \frac{\rho^{\circ}}{1-\rho^{\circ}\alpha t} \\ z+z^* &= z^*(1-\rho^{\circ}\alpha t)^2 \\ \psi &= -\alpha z^*(\rho^{\circ})^2 t \end{aligned}\right\} \tag{5.34}$$

or, upon inverting,

$$\psi(z,t) = -\frac{z^*}{\alpha t}\left(\left(\frac{z+z^*}{z^*}\right)^{1/2}-1\right)^2 \tag{5.35}$$

The "Jacobian" is simply the derivative

$$J = \frac{dz}{d\rho^0} = -2z^*\alpha t\,(1-\rho^0\alpha t) = -2z^*\alpha t\left(\frac{z+z^*}{z^*}\right)^{1/2}$$

and

$$A^{(0)}(t) \propto \frac{1}{|J|^{1/2}} = \frac{1}{(2z^*\alpha t)^{1/2}}\left(\frac{z^*}{z+z^*}\right)^{1/4}$$

or

$$A^{(0)}(z,t) = \frac{1}{(4\pi z^*\alpha t)^{1/2}}\left(\frac{z^*}{z+z^*}\right)^{1/4} \tag{5.36}$$

Thus, the low order approximation to the solution is

$$C^{(0)} = \frac{\lambda^{1/2}}{(4\pi z^*\alpha t)^{1/2}}\left(\frac{z^*}{z+z^*}\right)^{1/4}\exp\left\{-\frac{\lambda z^*}{\alpha t}\left[\left(\frac{z+z^*}{z^*}\right)^{1/2}-1\right]^2\right\} \tag{5.37}$$

In obtaining higher order approximations, the computations become simpler if we relate the operator,

$$\frac{\partial}{\partial z}K\frac{\partial}{\partial z}A^{(n)}$$

with t fixed to a (ρ^0, t) coordinate system.

In such a system, we have

$$A^{(0)}(t) = \frac{1}{(4\pi z^*\alpha t)^{1/2}}\left(1-\rho^0\alpha t\right)^{-1/2}$$

while

$$\frac{\partial}{\partial z}\Big|_t = \frac{\partial\rho^0}{\partial z}\Big|_t\frac{\partial}{\partial\rho^0}\Big|_t = -\frac{1}{2z^*\alpha t}\frac{1}{(1-\rho^0\alpha t)}\frac{\partial}{\partial\rho^0}\Big|_t$$

Indeed, in a ($\rho^0\alpha t, t$) coordinate system, representing $\rho^0\alpha t = \varsigma$, we have

$$\frac{\partial}{\partial z}\Big|_t = -\frac{1}{2z^*}\frac{1}{1-\varsigma}\frac{\partial}{\partial\varsigma}\Big|_t$$

and

$$\frac{\partial}{\partial z}K\frac{\partial}{\partial z} = \frac{1}{2z^*}\frac{1}{1-\varsigma}\frac{\partial}{\partial\varsigma}\left[\alpha z^*(1-\varsigma)^2\cdot\frac{1}{2z^*}\frac{1}{1-\varsigma}\frac{\partial}{\partial\varsigma}\right]$$

$$= \frac{\alpha}{4z^*}\frac{1}{1-\varsigma}\frac{\partial}{\partial\varsigma}(1-\varsigma)\frac{\partial}{\partial\varsigma}$$

If we let $A^{(n)} = f^{(n)}A^{(0)}$, we have

$$\frac{\partial}{\partial z}K\frac{\partial}{\partial z}A^{(n)} = \frac{\alpha}{4z^*}\frac{1}{1-\varsigma}\frac{\partial}{\partial\varsigma}\left[(1-\varsigma)\frac{\partial}{\partial\varsigma}\left(f^{(n)}A^{(0)}\right)\right]$$

$$= \frac{\alpha}{4z^*}\frac{1}{1-\varsigma}\frac{\partial}{\partial\varsigma}\left[A^{(0)}(1-\varsigma)\frac{\partial f^{(n)}}{\partial\varsigma} + f^{(n)}(1-\varsigma)\frac{\partial A^{(0)}}{\partial\varsigma}\right]$$

$$= \frac{\alpha}{4z^*}\frac{1}{1-\varsigma}\left[A^{(0)}\frac{\partial}{\partial\varsigma}(1-\varsigma)\frac{\partial f^{(n)}}{\partial\varsigma} + 2(1-\varsigma)\frac{\partial f^{(n)}}{\partial\varsigma}\frac{\partial A^{(0)}}{\partial\varsigma} + f^{(n)}\frac{\partial}{\partial\varsigma}(1-\varsigma)\frac{\partial A^{(0)}}{\partial\varsigma}\right]$$

$$= \frac{\alpha}{4z^*}\frac{A^{(0)}}{1-\varsigma}\left[\frac{\partial}{\partial\varsigma}\left((1-\varsigma)\frac{\partial f^{(n)}}{\partial\varsigma}\right) + \frac{\partial(f^{(n)})}{\partial\varsigma} + \frac{1}{4}\frac{f^{(n)}}{(1-\varsigma)}\right]$$

$$= \frac{\alpha}{4z^*}A^{(0)}\left[\frac{\partial^2}{\partial\varsigma^2}f^{(n)} + \frac{1}{4}\frac{f^{(n)}}{(1-\varsigma)^2}\right]$$

Then, by (3.10),

$$A^{(n+1)} = A^{(0)}\left\{\int_0^t\left[A^{(0)}\right]^{-1}\frac{\partial}{\partial z}K\frac{\partial}{\partial z}\left[A^{(n)}\right]d\tau + C\right\}$$

$$= A^{(0)}\left\{\int_0^t\frac{\alpha}{4z^*}\left[\frac{\partial^2}{\partial\varsigma^2}f^{(n)} + \frac{1}{4}\frac{f^{(n)}}{(1-\varsigma)^2}\right]d\tau + C\right\}$$

or

$$f^{(n+1)} = \frac{\alpha}{4z^*}\int_0^t\left[\frac{\partial^2}{\partial\varsigma^2}f^{(n)} + \frac{1}{4}\frac{f^{(n)}}{(1-\varsigma)^2}\right]d\tau + C^{(n+1)}(\rho^0)$$

If we require that $f^{(n)}(z,t) = \frac{A^{(n)}(z,t)}{A^{(0)}(z,t)}$ be continuous at the z=0, t=0, then the constant of integration $C^{(n)}(p^0)$ must actually be the same for all rays emanating from the origin, and hence independent of p^0. If, moreover, the "strength" of the source as given by the first term $A^{(0)}$ is to be unaffected by each succeeding term, then all the $f^{(n)}$ must vanish at the origin, so the value of the integration constant must be zero.

Thus, $A^{(n)} = f^{(n)}A^{(0)}$, where

$$f^{(n+1)} = \int_0^t \frac{\alpha}{4z^*}\left[\frac{\partial^2}{\partial \zeta^2} f^{(n)} + \frac{1}{4}\frac{f^{(n)}}{(1-\zeta)^2}\right] d\tau \tag{5.38}$$

and $\zeta = \alpha t p^0$

Now $f^{(0)} \equiv 1$, so

$$f^{(1)} = \frac{1}{16 z^* p^0}\int_0^t \frac{\alpha p^0 \, d\tau}{(1-\alpha p^0 \tau)^2}$$

$$= \frac{1}{16 z^* p^0}\left[\frac{1}{(1-\alpha p^0 t)} - 1\right]$$

$$f^{(1)} = \frac{\alpha t}{16 z^* (1-p^0 \alpha t)} \tag{5.39}$$

$$f^{(2)} = \frac{\alpha^2}{64 z^{*2}}\int_0^t \tau\left[\frac{2}{(1-\alpha p^0 \tau)^3} + \frac{1}{4(1-\alpha p^0 \tau)^3}\right] d\tau$$

$$= \frac{1}{(16)^2 z^{*2} (p^0)^2}\int_0^t \frac{9\alpha p^0 \tau \, \alpha p^0 \, d\tau}{(1-\alpha p^0 \tau)^3}$$

$$f^{(2)} = \frac{9\alpha^2 t^2}{2\cdot(16)^2 z^{*2} (1-\alpha p^0 t)^2} \tag{5.40}$$

The remaining coefficients $f^{(n)}$ may be easily computed by assuming

$$f^{(n)} = K_n\left[\frac{\alpha \tau}{z^*(1-\alpha p^0 \tau)}\right]^n \tag{5.41}$$

Then we find

$$\frac{\partial^2}{\partial \zeta^2} f^{(n)} = K_n\left(\frac{\alpha \tau}{z^*}\right)^n \frac{-n(-n-1)}{(1-\alpha p^0 \tau)^{n+2}}$$

and

$$f^{(n+1)} = \int_0^t \frac{\alpha}{4z^*}\cdot K_n\left(\frac{\alpha \tau}{z^*}\right)^n\left[\frac{n(n+1)}{(1-\alpha p^0 \tau)^{n+2}} + \frac{1}{4(1-\alpha p^0 \tau)^{n+2}}\right] d\tau$$

$$= K_n\left(\frac{1}{p^0 z^*}\right)^{n+1}\frac{4(n+1)n+1}{16}\int_0^t \frac{(\alpha p^0 \tau)^n \, \alpha p^0 \, d\tau}{(1-\alpha p^0 \tau)^{n+2}}$$

$$= K_n\left(\frac{1}{p^0 z^*}\right)^{n+1}\frac{(2n+1)^2}{16(n+1)}\frac{1}{(1-\alpha p^0 t)^{n+1}}$$

$$= K_{n+1}\left[\frac{\alpha t}{z^*(1-\alpha p^0 t)}\right]^{n+1}$$

where

$$K_{n+1} = K_n \cdot \frac{1}{16}\frac{(2n+1)^2}{n+1} \tag{5.42}$$

or, since $K_0 = 1$

$$K_n = \frac{1}{16^n}\frac{1^2\cdot 3^2\cdot 5^2\cdots(2n-1)^2}{n!} \tag{5.43}$$

and

$$f^{(n)} = \frac{1}{16^n}\frac{1^2\cdot 3^2\cdot 5^2\cdots(2n-1)^2}{n!}\left[\frac{\alpha t}{z^*(1-\alpha p^0 t)}\right]^n. \tag{5.44}$$

$$= \frac{1}{16^n}\frac{1^2\cdot 3^2\cdot 5^2\cdots(2n-1)^2}{n!}\left[\frac{\alpha t}{z^*}\left(\frac{z^*}{z+z^*}\right)^{1/2}\right]^n$$

Thus

$$C(z,t) \approx \frac{\lambda^{1/2}}{(4\pi z^* \alpha t)^{1/2}} \left(\frac{z^*}{z+z^*}\right)^{1/4} \left\{ \sum_{n=0}^{\infty} \frac{\lambda^{-n}}{16^n} \frac{1^2 \cdot 3^2 \cdot 5^2 \cdots (2n-1)^2}{n!} \left[\frac{\alpha t}{z^*}\left(\frac{z^*}{z+z^*}\right)^{1/2}\right]\right\} \cdot \exp\left\{-\frac{\lambda z^*}{\alpha t}\left[\left(\frac{z+z^*}{z^*}\right)^{1/2}-1\right]^2\right\} \tag{5.45}$$

The asymptotic expansion in (5.45) converges nowhere, except trivially for t=0, but it may well be the asymptotic expansion of a function yielding the solution. Indeed, it appears to be the asymptotic expansion of a function $F(\zeta)$ where

$$\zeta = \frac{\lambda z^*}{\alpha t} \left(\frac{z+z^*}{z^*}\right)^{1/2} \tag{5.46}$$

Assuming this is the case, we may obtain F by assuming, from (2.7a)

$$C(z,t) = A(z,t;\lambda) \exp\{-\lambda \psi(z,t)\}$$

with

$$A(z,t;\lambda) = \lambda^{1/2} A^{(0)}(z,t)\, F(\zeta)$$

Then in place of (3.5a), (3.5b) we have

$$\frac{d}{dt} A = A \frac{\partial}{\partial z} K \frac{\partial \psi}{\partial z} + \lambda^{-1} \frac{\partial}{\partial z} K \frac{\partial A}{\partial z}$$

where $\frac{d}{dt}$ denotes differentiation along rays.

In view of (3.5a), we can then show

$$\frac{d}{dt} F(\zeta) = \lambda^{-1} \frac{\partial}{\partial z} K \frac{\partial F}{\partial z}$$

which leads to the differential equation for F:

$$F'' + 4F' + \frac{1}{4\zeta^2} F = 0$$

The solution to this equation is

$$F(\zeta) = \zeta^{1/2} e^{-2\zeta} \left[\beta I_0(2\zeta) + \gamma K_0(2\zeta)\right] \tag{5.47}$$

where β and γ are integration constants and I_0 and K_0 are modified Bessel's Functions of order zero. (Whittaker & Watson, pp. 273-274), (Erdelyi et. al. p. 5, 86).

The asymptotic expansions of these functions are

$$\zeta^{1/2} e^{-2\zeta} I_0(2\zeta) \sim \frac{1}{(4\pi)^{1/2}} \left[\sum_{n=0}^{\infty} \frac{1^2 \cdot 3^2 \cdot 5^2 \cdots (2n-1)^2}{n!\; 2^{3n}} \frac{1}{(2\zeta)^n}\right]$$

$$\zeta^{1/2} e^{-2\zeta} K_0(2\zeta) \sim \left(\frac{\pi}{4}\right)^{1/2} e^{-4\zeta} \left[1 + O(\zeta^{-1})\right]$$

$$\text{as } \zeta \to \infty \quad (\text{or } \lambda \to \infty)$$

The asymptotic expansion of (5.47) agrees with (5.45) for arbitrary values of γ, provided $\beta = (4\pi)^{1/2}$

In order to ascertain the value of γ, another boundary condition is needed. In view of the special nature of the line $z = -z^*$, where K becomes negative and the diffusion equation is inapplicable, it is reasonable to impose the boundary condition at that point. Now, the limit

$$F_\ell = \lim_{z \downarrow -z^*} K \frac{\partial C}{\partial z}$$

denotes the flux of the tracer across the line $z = -z^*$; we shall require that this flux vanish. This implies $\gamma = 0$, and the solution is

$$F(\zeta) = (4\pi)^{1/2} \zeta^{1/2} e^{-2\zeta} I_0(2\zeta)$$

The complete expression for the tracer density becomes

$$C(z,t;\lambda) = \lambda^{1/2} A^{1/2}(z,t)\, F(\zeta)\, \exp[-\lambda\, \psi(z,t)]$$
$$= \frac{\lambda}{\alpha t}\, I_0\left(\frac{2\lambda z^*}{\alpha t}\left(\frac{z+z^*}{z^*}\right)^{1/2}\right) \exp\left\{-\frac{2\lambda z^*}{\alpha t}\left(\frac{z+z^*}{z^*}\right)^{1/2}\right\}\cdot$$
$$\cdot \exp\left\{\frac{\lambda z^*}{\alpha t}\left[\left(\frac{z+z^*}{z^*}\right)^{1/2}-1\right]^2\right\}$$

or

$$C(z,t;\lambda) = \frac{\lambda}{\alpha t}\, I_0\left\{\frac{2\lambda z^*}{\alpha t}\left(\frac{z+z^*}{z^*}\right)^{1/2}\right\} \exp\left\{-\frac{\lambda(z+2z^*)}{\alpha t}\right\} \qquad (5.48)$$

for the exact solution to the point-source diffusion problem.

As already mentioned, (5.43) is an asymptotic expansion for the solution (5.48), and has the advantage of being easier to compare with the classical solution for diffusion.

Furthermore, in practical situations, the principal concern will be with regions where $t \ll \frac{\alpha}{\lambda z^*}$ and $|z| \ll |z^*|$; in short when

$$\zeta = \frac{\lambda z^*}{\alpha t}\left(\frac{z+z^*}{z^*}\right)^{1/2} \gg 1$$

Under these conditions, the first asymptotic approximation (5.37) will provide an adequate representation to the solution.

6. DISCUSSION

We have seen that the ray method in several cases leads directly to a useful approximation to the Green's function for dispersion problems involving diffusion and advection. Indeed, it occasionally

leads to new exact solutions for the Green's function. By integrating these solutions over a volume source, an approximation to the solution of this more general problem may be obtained.

In the event that the exact solution is obtained, integration over time will lead to the exact solution for a continuous, constant strength point source.

In the course of this paper, the domains chosen were free of boundaries, other than those required by singularities in the differential equation. However, if an impedance type boundary condition (a linear combination of C and its normal derivative are prescribed for all time) is chosen, it is possible to deal with this also. In this event, a second asymptotic expansion of the form (2.7b) would be assumed, and the solution C would be regarded as the sum of two expansions. The rays for the second expansion would emanate from the boundary, and initial data for its exponential and transport terms would be obtained from the boundary conditions on C. See (Keller and Rubinow, 1960), (Lewis, 1964) for further details.

One unsettled question which may be of interest deals with the meaning of the conserved quantity Q of equation (3.9). In geometrical optics, this term is the square of the wave amplitude and related to the energy transported along the ray, but in diffusion it is not clear whether Q is related to any physical quantity. It would seem strange if a quantity conserved in an asymptotic approximation were not related to a conservative physical quantity.

There does not seem to be any complete answer to the question whether the expansions derived in this paper will, in general, be asymptotic to the solutions. The justification for their use lies primarily in the success with which they have been applied to problems in other fields. The examples shown in section 5 provide encouraging evidence of the utility of these expansions in the present case as well.

Of great importance in any asymptotic expansion is the problem of the uniformity of the expansion. That is, for any given level of accuracy, can a value of λ be chosen so the approximations are accurate to this level for all space and time? If not, in what regions will this hold true? In particular, is there a region of uniformity containing the source, either as interior or boundary point?

Again, the theoretical background is lacking for a complete answer to these questions. However, some insight may be attained by examining the examples which we have derived.

In general, it seems that if the expansions do not truncate and thereby yield the exact solution, they are not uniform over all space-time. But there exist regions in which they are uniform, and these regions in general are separated from those loci where the rays converge, known as "caustics". Particular caustics include

"point sources", and, in example C, section 5, the line $z+z^* = 0$, which is a singularity of the differential equation. In the classical applications of ray theory, the regions of uniformity are separated from the point source. For example, in geometrical optics and acoustics, one is concerned with the reduced wave equation $(\nabla^2 + k^2)\, u = 0$ (Jeffreys, 1962), (Friedlander and Keller, 1955), (Keller and Rubinow, 1960), (Lewis and Keller, 1963). If the index of refraction, k, is constant, then for spaces whose number of dimensions is odd, the ray theory approximations truncate to the exact solution, but for even dimensioned spaces, the exact solutions have logarithmic singularities at the source, where the ray theory approximations have simply poles. Thus, in this case, either the expansion truncates to the exact solution, or it is not valid in the near neighborhood of the source.

By contrast, for the last example in section 5, the expansion is uniform in regions of the type $0 < t < M(z+z)^{\frac{1}{2}}$ for all constants M, and each of these regions include the source. This welcome feature may be a consequence of the parabolic nature of the original equations.

Among the benefits of ray procedures are their adaptability to machine computation. The basis for the computation of the exponential and the transport terms is the integration of systems of ordinary differential equations, and the literature is rife with methods, such as the Runge-Kutta and the predictor-corrector methods, for doing this numerically.

The principal alternative procedure for integrating diffusion-advection equations numerically relies in the use of a fixed grid approximate the space-derivatives of C, use (2.5) to find the time derivative, and use the time derivative to find the next value of C at each point. Such a procedure has had success in a wide variety of different problems, but has one important limitation: it is unreliable in handling severe changes in gradient (Wurtele, 1961). The reason for this is that, when the solution undergoes rapid changes in higher order derivatives, more "mesh points" are required to resolve those changes. In the case of point-source diffusion, typically there are gradients of all sizes in any neighborhood of the source, if the time t is sufficiently small. Indefinitely many mesh points would be required, even in a scheme with variable mesh spacing.

On the other hand ray techniques would concentrate the computation points where the rays are concentrated, which in general would be in those areas and at those times where the solution itself undergoes the greatest changes, and so large gradients would be properly advected. The compensating drawback is that succeeding iterations do not even theoretically lead to an exact solution.

A combination of these two procedures would then seem to be a practical approach to machine solution of this type of problem. After the exponential argument ψ and the first transport term $A^{(o)}$ were obtained by the procedures in this paper, the remainder term would be computed by a finite difference scheme.

We could either represent

$$C = \lambda^{N/2} A^{(0)} A^{*} e^{\lambda\psi}$$

or

$$C = C^{(0)} + C^{*} \quad , \text{ where } , \quad C^{(0)} = \lambda^{N/2} A^{(0)} e^{\lambda\psi}$$

In the former case, A* would satisfy

$$\frac{dA^{*}}{dt} = \frac{1}{A^{(0)}} \frac{1}{\lambda} \frac{\partial}{\partial x_i} \left[K_{ij} \frac{\partial}{\partial x_j} (A^{*} A^{(0)}) \right]$$

where the initial value for A^{*} is identically unity. The grid system would be fixed in the ray coordinate system, since the time derivative is taken along the ray.

In the latter case, C* would satisfy

$$\frac{\partial C^{*}}{\partial t} + \frac{\partial}{\partial x_i}(u_i C^{*}) - \frac{1}{\lambda} \frac{\partial}{\partial x_i} K_{ij} \frac{\partial C^{*}}{\partial x_j} = \frac{1}{\lambda} e^{\lambda\psi} \frac{\partial}{\partial x_i} \left[K_{ij} \frac{\partial A^{(0)}}{\partial x_j} \right]$$

with vanishing initial data. In either case, the solutions could be expected to be much smoother than the solution to the original problem, and hence amenable to the rectangular grid approach.

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LEGENDS

Fig. 1. Rays and ray tubes in space-time.

Fig. 2. Rays and ray tubes from an instantaneous point source for the case of no advection and constant diffusion coefficients.

Fig. 3. Projections of selected rays on the x-y plane for the case of linear shear flow (u=by). Rays leaving the origin in the first quadrant depart in the same direction, but at different speeds, while those in the other quadrants have a common speed, but depart in different directions. All the rays curve in the direction of rotation of the main flow.

Fig. 4. Streamlines and projections of rays for the case of hyperbolic bilinear shear flow ($u = \omega_1 y$, $v = \omega_2 x$, $\omega_1 > 0, \omega_2 > 0$). All rays curve in the direction of the (constant) rotation of the flow, asymptotically tending to parallel the downstream asymptotes of the streamlines.

Fig. 5. Streamlines and projections of rays for elliptic bilinear shear flow ($u = \omega_1 y$, $v = \omega_2 x$, $\omega_1 < 0$, $\omega_2 > 0$).

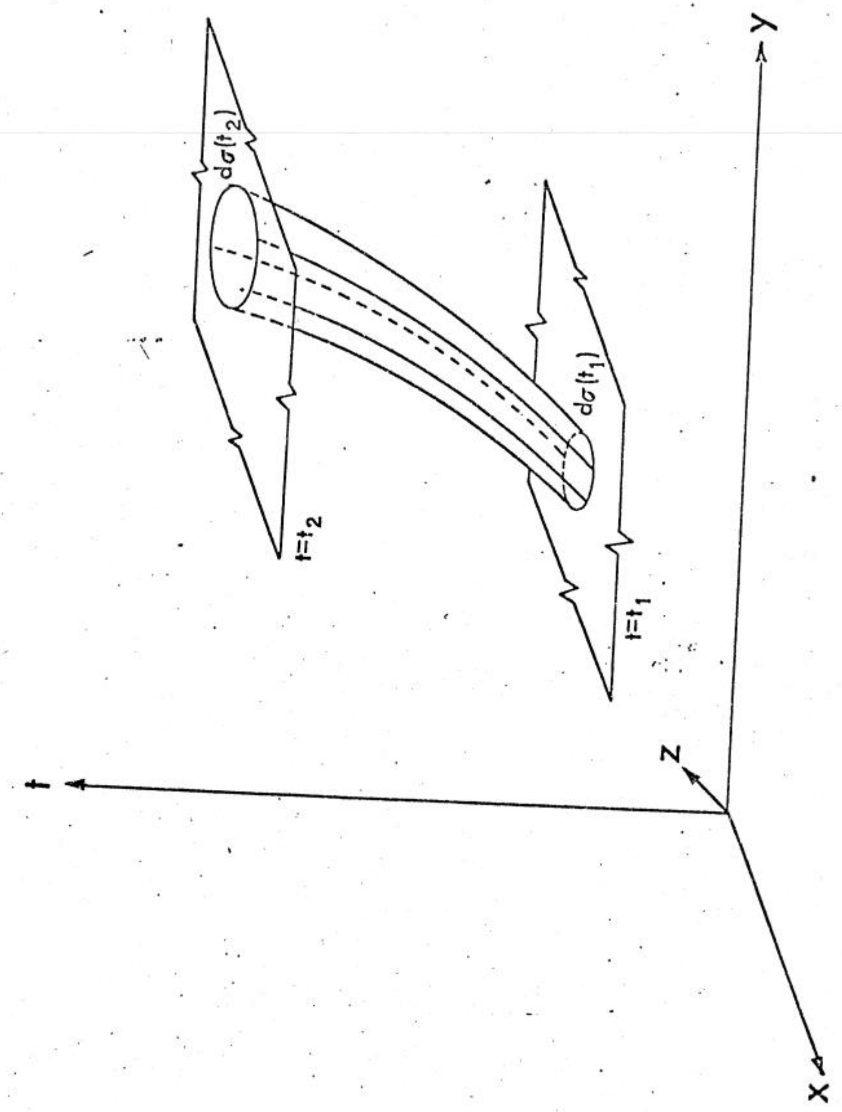

FIGURE 1

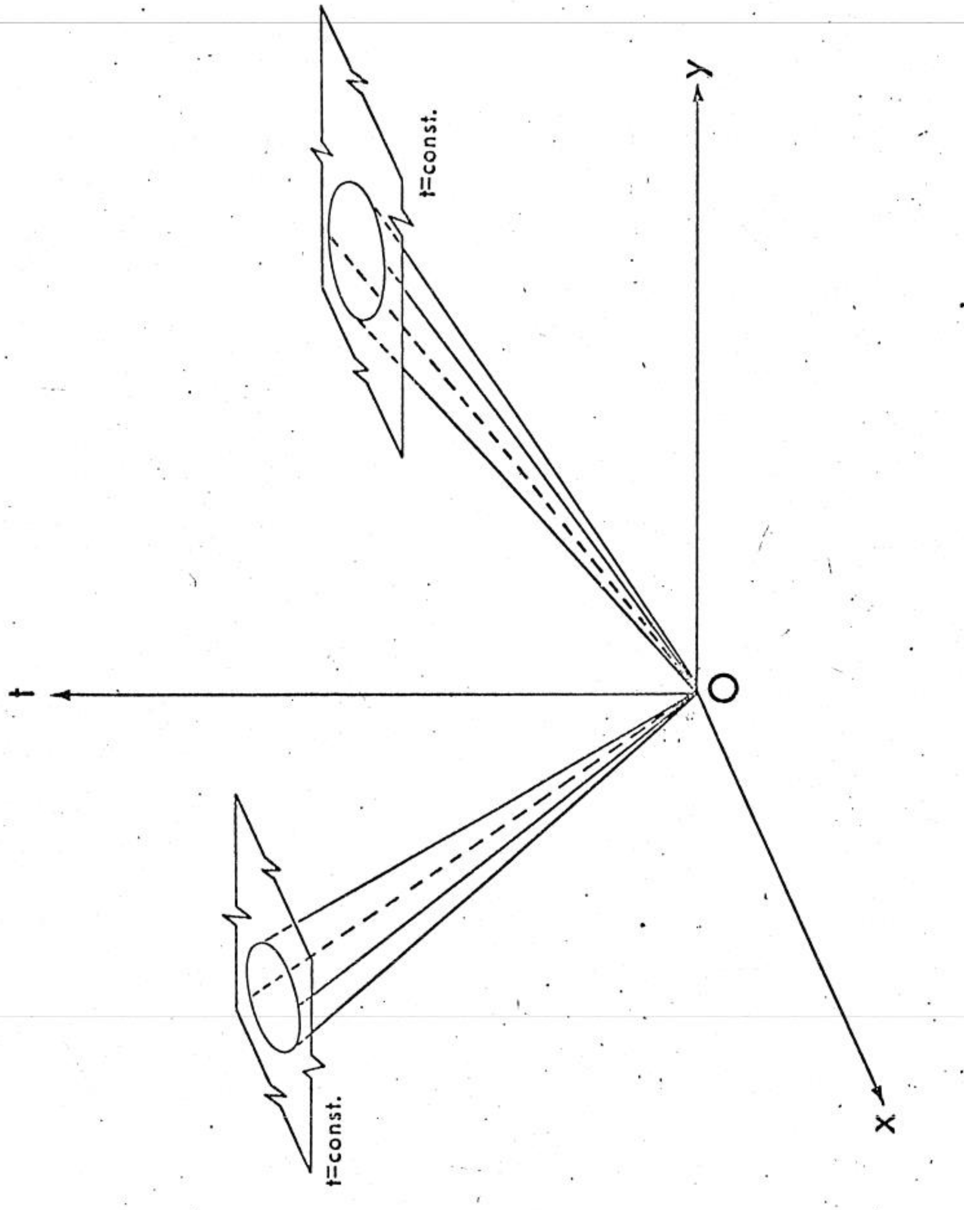

FIGURE 2

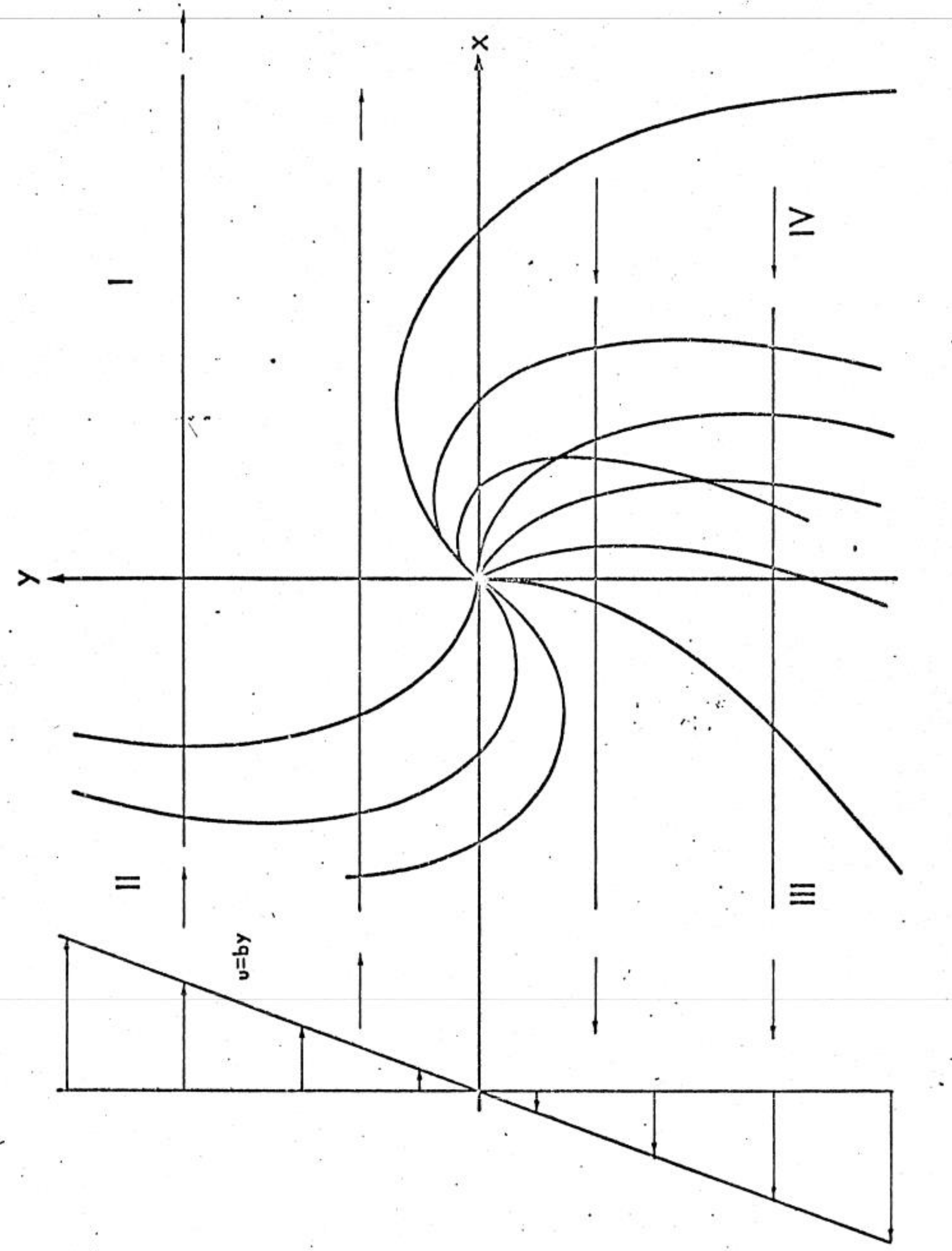

FIGURE 3

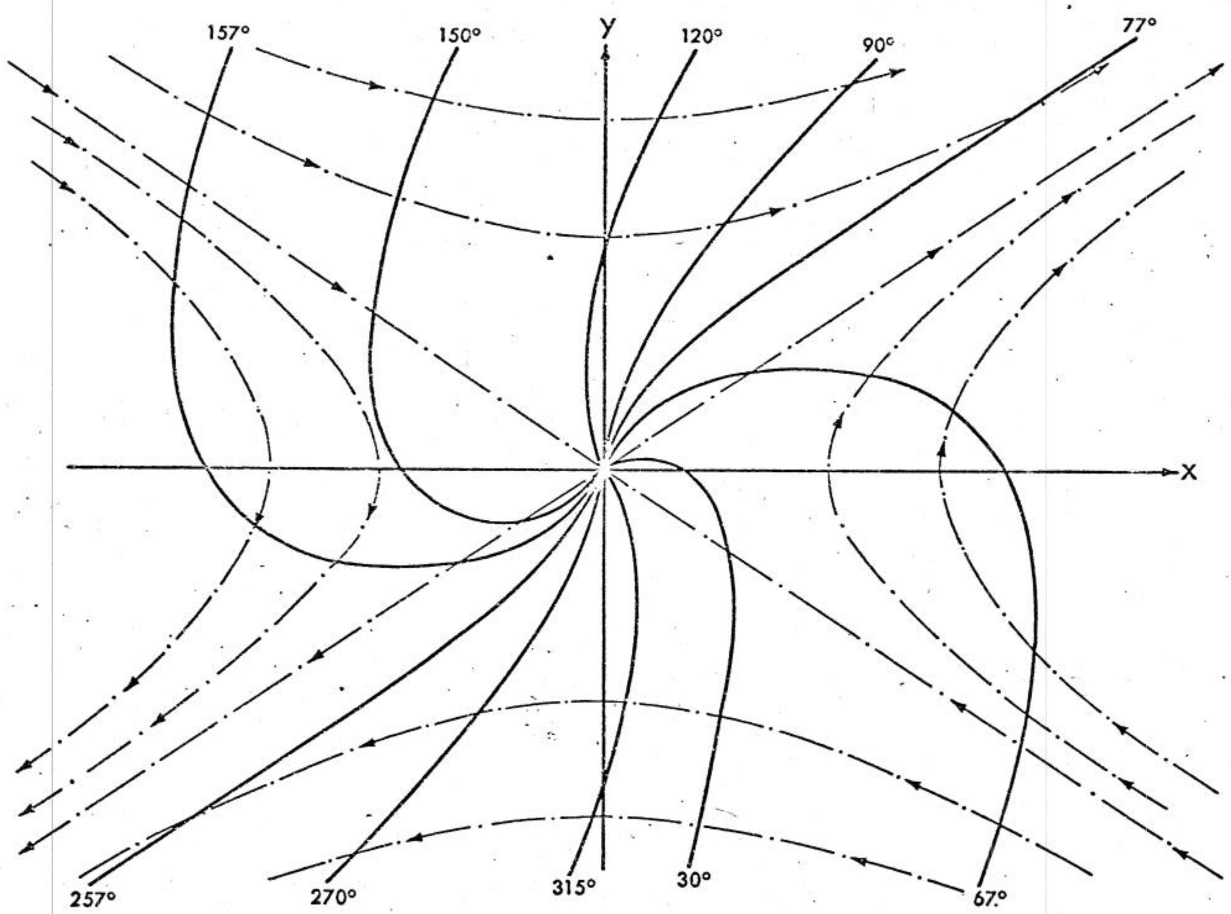

FIGURE 4

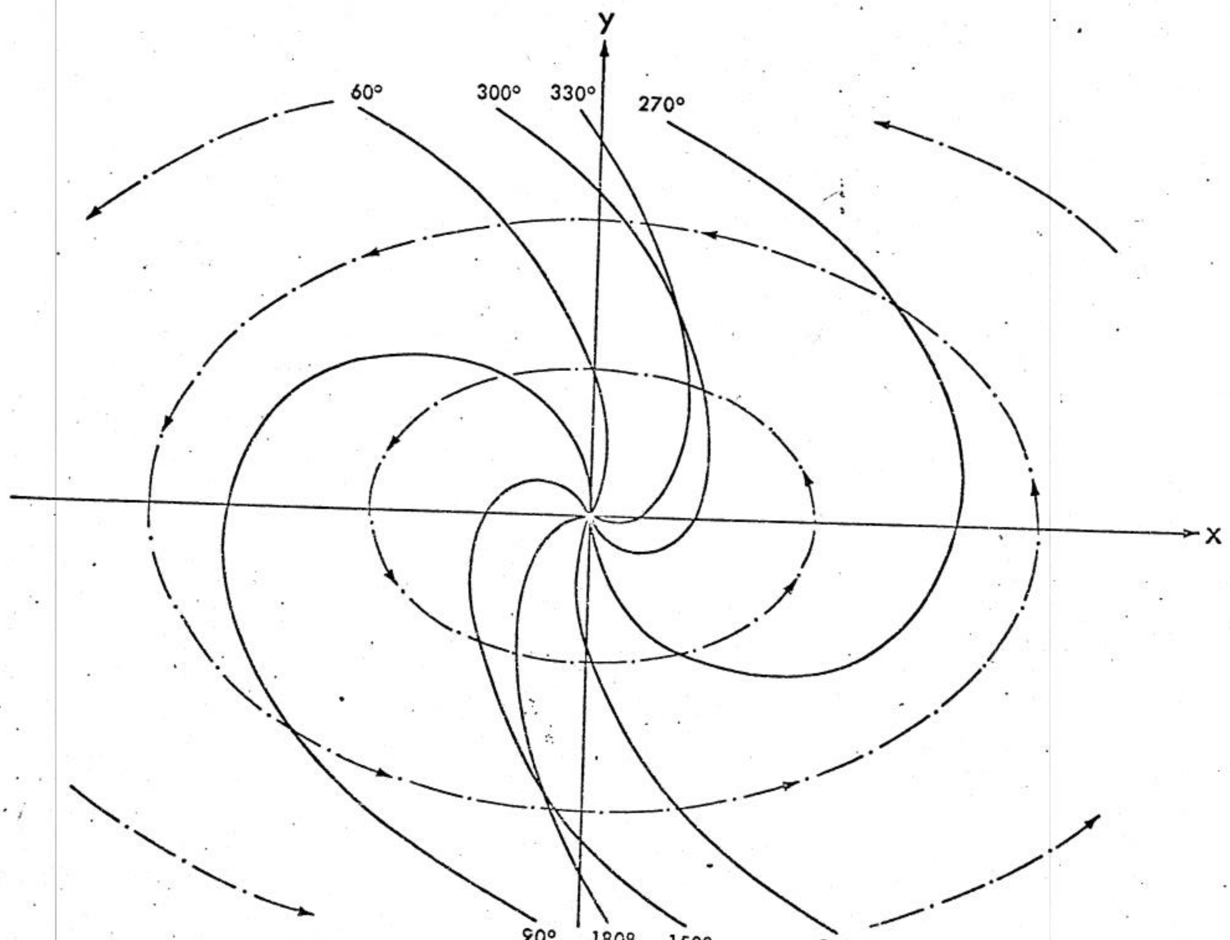

FIGURE 5