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INFLUENCE OF MOLECULAR DIFFUSIVITY ON DIFFUSION FROM AN INSTANTANEOUS POINT SOURCE IN A UNIFORM, TIME DEPENDENT VELOCITY FIELD

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Abstract—The exact solution of the difiusion equation for an instantaneous point source in a uniform, time dependent, velocity field is found. This solution contains Taylor's theory of diffusion by continuous movements as a particular case, which is discussed. Influence of molecular diffusivity is assessed.

NOMENCLATURE

c,	mass concentration, temperature, enthalpy;
F_1, F_2, F_3,	defined by (14);
I,	$= \sqrt{(-1)}$;
$\kappa_1, \kappa_2, \kappa_3$,	wave vector in Fourier space;
κ^2,	modulus squared of wave vector;
r_1, r_2, r_3,	separation vector ($r_j = x_j - x_j'$);
t,	non-dimensional time;
U_1, U_2, U_3,	non-dimensional velocity components;
x_1, x_2, x_3,	cartesian coordinates;
$\langle\ \rangle$,	ensemble average.

Greek symbols

Υ,	velocity scale;
T,	time scale;
τ,	time difference;
ν,	non-dimensional molecular diffusivity for mass, temperature or enthalpy;
ν_t,	turbulent diffusivity;
ρ,	autocorrelation coefficient defined by (5);
δ,	Dirac delta function;
Π,	product.

Superscripts

$*$,	denotes dimensional form;
$'$,	coordinates of another point;
$\hat{}$,	three-dimensional Fourier transform.

Subscripts

i, j, m,	coordinate index ($i, j, m = 1, 2, 3$) repeated subscript means summation on that index.

1. INTRODUCTION

DIFFUSION of enthalpy or chemical species in a turbulent field have deserved much less theoretical attention than the turbulent flow itself. The reason seems obvious: since the fundamental problems of turbulent flows are not yet solved, and as the whole of the theory still rests on more or less empirical assumptions and physical inputs (at one or other level), it does not appear to be of much use as a theory of diffusion for enthalpy or chemical species which have the knowledge of the turbulent field as an essential input. There are, however, several reasons for not taking the obvious for granted. Among these are: (a) mathematically, the diffusion equation is of the same type as the momentum equations, but simpler, because it is linear in the unknowns; (b) the use of tracers is still largely used for the experimental study of the turbulent flow itself; (c) diffusion of enthalpy or chemical species, is an extremely important problem in itself, which suffers in its practical applications from the effects of a double set of assumptions and empiricisms: those associated with the flow and the additional ones from the diffusion.

The mathematical similarity of momentum and species (or enthalpy) diffusion is in fact implied in the engineering approaches to the computation of heat and mass transfer through the concept of Prandtl or Schmidt numbers mainly when used in connection with well known "models of turbulence". However, that physical similarity in the way which is usually done in engineering is only mathematically supported to a limited extent. Mathematics says that it can only be so when $\nu \sim 1$ and when both fields are already dominated by the influence of a uniform boundary condition. This inference is supported by experiment and clearly points out that a search for experimentally based correlation of turbulent Prandtl or Schmidt numbers in the general situations of three-dimensional flows will probably lead to a dead end. In the best experimentally known flow situations, like free turbulent boundary-layers, reaction or simply diffusion of chemical species with widely different molecular diffusivities, or varying boundary conditions complicates the usual treatments.

In this paper a different approach is taken. It aims at a clarification of the interplay between the physical inputs regarding the turbulent flow and the mathematical implications on the turbulent diffusion of enthalpy or chemical species. In a sense, the present results generalise those of Taylor's pioneering paper [1], by taking into account molecular diffusivity; therefore, the present results have engineering relevance in problems of polutant dispersion, where Taylor's results are widely used. On a wider sense, subsequent work will show how this type of approach is useful in the development of computational models of turbulence.

Generally speaking, for contaminant diffusion in turbulent flows, the approximation of neglecting ν is certainly acceptable if only one contaminant is present. However, if more than one contaminant is present and the relative values of their concentration is important, their respective diffusivities must be taken into account. For instance, the relation between ν for H_2 and O_2 in air is ~4.3. The relation will increase with the ratio of molecular weights, and certainly must be considered if their chemical reaction is the main concern.

2. OUTLINE OF THE MAIN CONTRIBUTION

The present results apply to an unbounded flow field and an instantaneous point source, assuming as a starting point the fundamental partial differential equation for the diffusion of enthalpy or chemical species. The flow field is assumed spatially uniform and arbitrarily time dependent. Extension to non-uniform shear flows is, however, mathematically straightforward because the fundamental solution obtained can be extended by the parametrix method to any arbitrarily space and time dependent flow.

The general solution is obtained in closed form as a definite integral whose integrand is the analytical expression of the flow field. The physical input enters at this level in the form of an assumed probability distribution. This distribution is assumed gaussian. If the velocity components are also assumed statistically independent a generalization of Taylor results with inclusion of molecular effects is obtained. These are particularly useful when more than one chemical species are present. Further, it is shown that, with all the above restrictions, the ensemble average concentration, when $t \to \infty$, is the solution of a heat conduction type equation $\partial c/\partial t = \nu_t \nabla^2 c$ with a well defined expression for the turbulent diffusivity ($\nu_t = 2\langle u_j u_j \rangle$). This, however, is more the exception than the rule: other types of probability distribution or the inclusion of shear effects cannot be reduced in general to a meaningful and generally valid Prandtl or Schmidt number.

3. FUNDAMENTAL SOLUTION

The concentration of a passive contaminant on a uniform velocity field $U_j^*(t)$ is given by:

$$\frac{\partial c}{\partial t^*} + U_j^* \frac{\partial c}{\partial x_j^*} = \nu^* \frac{\partial^2 c}{\partial x_j^* \partial x_j^*} \tag{1}$$

the molecular diffusivity ν^* is assumed constant. $U_j^*(t^*)$ will be subject to the condition

$$\langle U_j^* \rangle = 0. \tag{2}$$

Equation (1) may be made non-dimensional with the help of two scales. These scales, Υ and T will be chosen such that

$$\Upsilon^2 = \lim_{t^* \to \infty} \left\{ \frac{1}{t^*} \int_0^{t^*} U_j^* U_j^* \, \mathrm{d}t^* \right\} \tag{3}$$

and

$$\mathrm{T} = \int_0^\infty \rho(\tau) \, \mathrm{d}\tau \tag{4}$$

where $\rho(\tau)$ is defined by

$$\rho(\tau) \times \langle U_j^*(t^*) \times U_j^*(t^*) \rangle = \langle U_j^*(t^*) \times U_j^*(t^* + \tau) \rangle. \tag{5}$$

Equation (1) when expressed in terms of the above defined non-dimensional quantities, becomes:

$$\frac{\partial c}{\partial t} + U_j \frac{\partial c}{\partial x_j} = \nu \frac{\partial^2 c}{\partial x_j \partial x_j} \tag{6}$$

where:

$$\left.\begin{aligned} t &= \frac{t^*}{\mathrm{T}} \\ x_j &= \frac{x_j^*}{\Upsilon \mathrm{T}} \\ U_j &= \frac{U_j^*}{\Upsilon} \\ \nu &= \frac{\nu^*}{\Upsilon^2 \mathrm{T}} \end{aligned}\right\}. \tag{7}$$

Equation (6) is solved subject to the initial condition

$$c(\mathbf{x}, t = 0) = \delta(\mathbf{x} - \mathbf{x}') \tag{8}$$

which corresponds to a zero concentration everywhere, except at $\mathbf{x} = \mathbf{x}'$.

Integration of equation (8) may be achieved using a three-dimensional integral Fourier Transform

$$\hat{c} = \iiint_{-\infty}^{\infty} \exp\{I\kappa_j x_j\} \cdot c(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \tag{9}$$

$$c = \frac{1}{(2\pi)^3} \iiint_{-\infty}^{\infty} \exp\{-I\kappa_j x_j\} \cdot \hat{c}(\boldsymbol{\kappa}, t) \, \mathrm{d}\boldsymbol{\kappa} \tag{10}$$

where

$$I = \sqrt{(-1)}.$$

Introducing (10) in (6) yields

$$\frac{\partial \hat{c}}{\partial t} + (\nu\kappa^2 + I\kappa_j U_j)\hat{c} = 0 \tag{11}$$

whose solution is

$$\begin{aligned} \hat{c} &= \hat{\delta} \exp\left\{ -\int_0^t (\nu\kappa^2 + I\kappa_j U_j) \, \mathrm{d}t \right\} \\ &= \exp\left\{ -I\kappa_j x_j' - \int_0^t (\nu\kappa^2 + I\kappa_j U_j) \, \mathrm{d}t \right\}. \end{aligned} \tag{12}$$

Inverting the transformation

$$c = \frac{1}{(2\pi)^3} \iiint_{-\infty}^{+\infty} \exp\{-\nu t \kappa^2 + I\kappa_j[(x_j - x_j') - F_j(t)]\} \, \mathrm{d}\boldsymbol{\kappa} \tag{13}$$

where:

$$F_j(t) = \int_0^t U_j(t') \, \mathrm{d}t'. \tag{14}$$

Performing the integration over the space $\boldsymbol{\kappa}$, equation (13) becomes (see Appendix)

$$c = \frac{1}{(4\pi\nu t)^{3/2}} \exp\left\{ -\frac{1}{4\nu t}[r_j - F_j][r_j - F_j] \right\} \quad (15)$$

where r_j is the separation vector, $r_j = x_j - x_j'$.

Equation (15) is the fundamental solution, whose expression depends on $F_j(t)$.

4. MEAN VALUES FOR GAUSSIAN AND UNCORRELATED $F_j(t)$

The mean value of c may be obtained by ensemble averaging (15). If F_1, F_2, F_3 are assumed Gaussian and uncorrelated, the probability density distribution of F_j is given by:

$$P(F_1, F_2, F_3) = \frac{1}{(2\pi)^{3/2}} \frac{1}{\sigma_1\sigma_2\sigma_3} \exp\left\{ -\frac{F_1^2}{2\sigma_1^2} - \frac{F_2^2}{2\sigma_2^2} - \frac{F_3^2}{2\sigma_3^2} \right\}. \quad (16)$$

The quantities σ_1, σ_2 and σ_3 are the variances of F_1, F_2 and F_3, respectively. Ensemble averaging equation (15) and using relation (16), $\langle c \rangle$ is given by:

$$\langle c(\mathbf{x}, \mathbf{r}, t) \rangle = \frac{1}{(4\pi\nu t)^{3/2}} \frac{1}{(2\pi)^{3/2}} \times \prod_{m=1}^{3} \frac{1}{\sigma_m} \exp\left\{ -\frac{r_m r_m}{4\nu t} \right\} \times \int_{-\infty}^{+\infty} \exp\left\{ -\left[\frac{1}{4\nu t} + \frac{1}{2\sigma_m^2} \right] F_m F_m + \frac{F_m r_m}{2\nu t} \right\} \mathrm{d}F_m \quad (17)$$

(note that repeated index, m, does not represent summation).

Noting that ([2], p. 307)

$$\int_{-\infty}^{+\infty} \exp\{-px^2 \pm qx\}\,\mathrm{d}x = \left(\frac{\pi}{p}\right)^{1/2} \exp\left\{\frac{q^2}{4p}\right\}, \quad (18)$$

equation (17) yields:

$$\langle c \rangle = \frac{1}{\pi^{3/2}} \frac{1}{\{(4\nu t)^3 + 2(4\nu t)^2(\sigma_1^2 + \sigma_2^2 + \sigma_3^2) + 4(4\nu t)(\sigma_2^2\sigma_3^2 + \sigma_3^2\sigma_1^2 + \sigma_1^2\sigma_2^2) + 8\sigma_1^2\sigma_2^2\sigma_3^2\}^{1/2}} \times \exp\left\{ -\frac{r_1^2}{2\sigma_1^2 + 4\nu t} - \frac{r_2^2}{2\sigma_2^2 + 4\nu t} - \frac{r_3^2}{2\sigma_3^2 + 4\nu t} \right\}. \quad (19)$$

Since the field is assumed uniform, $\sigma_j = \sigma_j(t)$. Furthermore, the summation of the σ_j^2 satisfies the following limiting conditions:

$$\sum_{j=1}^{3} \sigma_j^2 = 2\Upsilon^2 t^2 \quad \text{for} \quad t \to 0 \quad (20)$$

$$\sum_{j=1}^{3} \sigma_j^2 = 2\Upsilon^2 \mathrm{T} t \quad \text{for} \quad t \to \infty. \quad (21)$$

For any value of t,

$$\sum_{j=1}^{3} \sigma_j^2$$

is known, provided the autocorrelation ρ (equation 5) is known.

Equation (19) shows that for high Reynolds numbers (i.e. $\nu \approx 0$), the influence of molecular diffusivity is very small. Furthermore, for $t \to \infty$, the solution coincides with that of $\partial c/\partial t = \nu_t \nabla^2 c$, with $\nu_t = 2\Upsilon^2\mathrm{T}$.

All the above results apply to the situation where $\langle U_j \rangle = 0$. However, if $\langle U_j \rangle$ is different from zero, the results may be applied to a coordinate system moving with a constant velocity $\langle U_j \rangle$. Extension to a time dependent $\langle U_j \rangle$ is restricted to situations when the time scales of the motion $\langle U_j \rangle$ are sufficiently high when compared with T.

5. FINAL REMARKS AND CONCLUSIONS

The main result is expressed by (15). Expression (19) embodies two fundamental assumptions: Gaussian distribution and uncorrelation of the F_j among themselves. Those assumptions with the additional one of $\nu \to 0$ set the limitations of Taylor's theory, within the framework of the fundamental diffusion equation.

Gaussian distribution of the F_j, can be formally deduced from the assumption of Gaussian distribution of the U_j only when $t \to \infty$; such inference is plausible on physical grounds. A mathematical proof is not known to us.

Within the intrinsic assumptions of Taylor's theory, result (19) shows the influence of finite ν, however small. This influence is likely to be practically relevant when chemical species with different ν are present, mainly when reaction among themselves is important.

From the above results, it becomes clear that the existence of a turbulent diffusivity will be more the exception than the rule, at least in rigorous terms. In fact, only when the above referred assumptions are acceptable and when $t \to \infty$ does such a turbulent diffusivity have a formal meaning.

Some of the limitations which are implied in (19) are easily removed. The most straightforward is the independence of the F_j. If they are assumed Gaussian, taking into account their correlation only amounts to a (very) tedious work to arrive at an exact final expression. Assumption of other types of distribution is done starting from (15).

From a practical point of view, one of the first extensions comes from an assumption of a form for ρ, taking into account the limiting cases of $t = 0$ and $t = \infty$.

Important, either from a theoretical or a practical point of view is the inclusion of shear effects. This is done using the fundamental solution (15) and the parametrix method. This is an iterative method, which essentially consists in taking (15) as the starting iteration. Proceeding in this way, the first iteration shows already the effect of shear.

As a final conclusion, the reported results, besides their own interest, are considered mainly important by the new lines of research they uncover.

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2. I. S. Gradshteyn and I. W. Ryzhik, *Table of Integrals, Series and Products.* Academic Press, New York (1965).

APPENDIX

Introducing

$$Z_j = [(x_j - x_j') - F_j(t)] = r_j - F_j(t)$$

(13) can be written

$$c = \frac{1}{(2\pi)^3}\iiint_{-\infty}^{\infty} \exp\{-(\nu t\kappa^2 + I\kappa_j Z_j)\}\,\mathrm{d}\boldsymbol{\kappa}$$

$\kappa_j Z_j$ is the inner product of the vectors $\boldsymbol{\kappa}$ and $\mathbf{Z}$, whose value is

$$\kappa_j Z_j = |\boldsymbol{\kappa}||Z|\cos\theta$$

where θ is the angle between them.

But

$$|\boldsymbol{\kappa}| = \sqrt{(\kappa_1^2 + \kappa_2^2 + \kappa_3^2)} = R$$

$$|\mathbf{Z}| = \sqrt{(Z_1^2 + Z_2^2 + Z_3^2)}.$$

Introducing a coordinate rotation in $\boldsymbol{\kappa}$ space to make $0x_3$ coincident with the direction of vector $\mathbf{Z}$, taking into account that the Jacobian of the transformation is 1, and introducing spherical coordinates (13) is transformed into

$$c = \frac{1}{(2\pi)^3}\int_0^\infty \mathrm{d}R \int_0^\pi \mathrm{d}\theta \times \int_0^{2\pi} \exp\{-(\nu t R^2 + IR|Z|\cos\theta)\}R^2 \sin\theta\,\mathrm{d}\phi$$

$$= \frac{2\pi}{(2\pi)^3}\int_0^\infty \exp\{-\nu t R^2\}R^2\,\mathrm{d}R \times \int_0^\pi \exp\{IR|Z|\cos\theta\}\sin\theta\,\mathrm{d}\theta.$$

Now

$$\int_0^\pi \exp\{IR|Z|\cos\theta\}\sin\theta\,\mathrm{d}\theta = \frac{2}{IR|Z|}\sinh(IR|Z|)$$

$$= \frac{4\sin(R|Z|)}{R|Z|}$$

and

$$c = \frac{1}{\pi^2|Z|}\int_0^\infty \exp\{-\nu t R^2\}R\sin(R|Z|)\,\mathrm{d}R.$$

In [2], p. 480, the following result can be found:

$$H = \int_0^\infty \exp\{-\beta R^2\}\cos(bR) = \tfrac{1}{2}\left(\frac{\pi}{\beta}\right)^{1/2}\exp\left(-\frac{b^2}{4\beta}\right).$$

From which:

$$-\frac{\mathrm{d}H}{\mathrm{d}b} = \int_0^\infty \exp\{-\beta R^2\}R\sin(bR) = \frac{b}{4\beta}\left(\frac{\pi}{\beta}\right)^{1/2}\exp\left\{-\frac{b^2}{4\beta}\right\}$$

putting $\beta = \nu t$; $b = |\mathbf{Z}|$ and introducing in c results:

$$c = \frac{1}{(4\pi\nu t)^{3/2}}\exp\left\{-\frac{1}{4\nu t}[r_j - F_j(t)][r_j - F_j(t)]\right\}$$

which is (15).

INFLUENCE DE LA DIFFUSIVITE MOLECULAIRE SUR LA DIFFUSION A PARTIR D'UNE SOURCE PONCTUELLE INSTANTANEE SITUEE DANS UN CHAMP DE VITESSE UNIFORME ET FONCTION DU TEMPS

Résumé—On donne la solution exacte de l'équation de la diffusion pour une source ponctuelle instantanée située dans un champ de vitesse uniforme et dépendant du temps. Cette solution contient comme cas particulier la théorie de Taylor de la diffusion par mouvements continus faisant l'objet d'une discussion. L'influence de la diffusivité moléculaire est déterminée.

DER EINFLUSS DES MOLEKULAREN DIFFUSIONSKOEFFIZIENTEN AUF DIE DIFFUSION VON EINER MOMENTANEN PUNKTQUELLE IN EIN GLEICHFÖRMIGES, ZEITABHÄNGIGES GESCHWINDIGKEITSFELD

Zusammenfassung—Es wird die exakte Lösung der Diffusionsgleichung für den Fall der Diffusion von einer momentanen Punktquelle in ein gleichförmiges, zeitabhängiges Geschwindigkeitsfeld abgeleitet. Die Lösung enthält als Spezialfall die Taylor-Theorie für die Diffusion durch kontinuierliche Bewegungen, welche diskutiert wird. Der Einfluß des molekularen Diffusionskoeffizienten wird abgeschätzt.

ВЛИЯНИЕ КОЭФФИЦИЕНТА МОЛЕКУЛЯРНОЙ ДИФФУЗИИ НА ПРОЦЕСС ДИФФУЗИИ ОТ МГНОВЕННОГО ТОЧЕЧНОГО ИСТОЧНИКА В ОДНОРОДНОМ ЗАВИСЯЩЕМ ОТ ВРЕМЕНИ ПОЛЕ СКОРОСТИ

Аннотация — Найдено точное решение уравнения диффузии для мгновенного точечного источника в однородном зависящем от времени поле скорости. Как частный случай, рассматриваемый в статье, решение включает разложение Тейлора для непрерывной диффузии. Подтверждено влияние коэффициента молекулярной диффузии.