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A PROGRESS REPORT ON MEAN GRADIENT HEAT TRANSFER IN ISOTROPIC TURBULENCE

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FOREWORD

An earlier version of this report was submitted in June 1968 to the Department of Chemical Engineering at the University of Washington, Seattle, Washington. Part of this report was prepared while the author was a Research Associate in that department.

MEAN GRADIENT HEAT TRANSFER IN ISOTROPIC TURBULENCE

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ABSTRACT

The problem of heat transfer of a constant-property fluid in isotropic turbulence in the presence of a uniform mean temperature gradient is examined. Three closures of the statistical moment equations are discussed: the first-iteration approximation, the third-cumulant discard, and the direct-interaction approximation. Evaluation of the thermal eddy diffusivity for the direct-interaction approximation requires solution of a nonlinear integro-differential equation for the averaged Green's function $\langle G \rangle$ for the temperature field. The numerical approximation of $\langle G \rangle$ was attempted in spatial coordinates to gain experience for shear-flow problems and so far is unsuccessful because of numerical difficulties associated with the singular nature of $\langle G \rangle$ at zero time. The calculation can best be done in wavenumber coordinates in which the Fourier transform of $\langle G \rangle$ is initially unity.

CONTENTS

MEAN GRADIENT HEAT TRANSFER IN ISOTROPIC TURBULENCE

1. INTRODUCTION

The problem treated here* is the calculation of the steady-state mean heat transfer rate for a specified uniform mean temperature gradient superimposed on a steady isotropic turbulent velocity field with known low-order statistics (e.g., space-time velocity covariance). The fluid is incompressible and has constant physical and thermal properties. The temperature field is passive, and viscous dissipation is negligible.

We denote statistical averages (ensemble averages) by angular brackets, so that the temperature and velocity fields for any realization are written $T(\mathbf{x},t) = \langle T(\mathbf{x},t)\rangle + \theta(\mathbf{x},t)$ and $\mathbf{U}(\mathbf{x},t) = \langle \mathbf{U}(\mathbf{x},t)\rangle + \mathbf{u}(\mathbf{x},t)$ where θ and $\mathbf{u}$ are the fluctuating or random parts of the fields. The heat equation for $\langle T\rangle$ reduces to $\langle \mathbf{u}\theta\rangle$ = constant vector, whose value is some function of $\nabla\langle T\rangle$ and of the statistics of the velocity field. For the present work we wish to determine the eddy diffusivity tensor κ^t, defined by $\langle \mathbf{u}\theta\rangle = -\kappa^t \cdot \nabla \langle T\rangle$, by making statistical or dynamical assumptions about the interaction between the velocity and temperature fields. In this report several such assumptions are discussed, the most interesting to us being Kraichnan's direct-interaction approximation,[1, 2, 3] which has not yet been studied for turbulent transport of a passive scalar by a mean gradient. Also, the problem is to be done in physical coordinates, with the idea of generalizing numerical techniques to shear-flow problems.†

Although this problem is rather idealized, data are available for a grid-generated turbulent flow heated to a self-maintained uniform temperature gradient.[4]

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*Suggested by Prof. C. A. Sleicher.

†The theories treated here, including the direct-interaction approximation, are set up in terms of Green's functions which have singular behavior at zero time in the spatial representation. In the wave-number or Fourier representation the singularity does not occur but, unfortunately, for non-homogeneous turbulence the Fourier representation requires a larger number of convolution integrals.

2. THEORY

For the general heat transfer problem (transient, non-homogeneous) let $\mathcal{L}$ be the operator

$$\mathcal{L} = \frac{\partial}{\partial t} + \langle \mathbf{U} \rangle \cdot \nabla - \kappa \nabla^2$$

where κ is the molecular thermal diffusivity. Then the instantaneous temperature field satisfies $\mathcal{L}T(\mathbf{x},t) = -\mathbf{u}(\mathbf{x},t) \cdot \nabla T(\mathbf{x},t)$ subject to suitable initial and boundary conditions. In terms of the Green's function[5] $G(\mathbf{x},t\,|\mathbf{x}',t')$ for response of the temperature field at $(\mathbf{x},t)$ to delta-function initial conditions, $G = \delta(\mathbf{x}-\mathbf{x}')$ at $t = t'$, and zero boundary conditions, $G = 0$ for $\mathbf{x}$ or $\mathbf{x}' \in \mathcal{B}$, the solution for arbitrary initial conditions $T_0(\mathbf{x}):\mathbf{x} \in \mathcal{R}$ and Dirichlet boundary conditions $T_B(\mathbf{x},t):\mathbf{x} \in \mathcal{B}$ is

$$T(\mathbf{x},t) = \int_{\mathcal{R}} G(\mathbf{x},t\,|\,\mathbf{x}',t_0)\,T_0(\mathbf{x}')\,d^3\mathbf{x}' - \kappa \int_{\mathcal{B}} \int_{t_0}^{t} T_B(\mathbf{x}',t') \frac{\partial}{\partial n'} G(\mathbf{x},t\,|\,\mathbf{x}',t')\,dt'\,d^2\mathbf{x}'$$

where $\mathbf{n}$ is the outward normal unit vector on $\mathcal{B}$. A similar treatment can be made for Neumann or Churchill boundary conditions. We shall use the above equations in a more symbolic notation with arguments $0 \Rightarrow (\mathbf{x},t)$, $1 \Rightarrow (\mathbf{x}',t')$, $2 \Rightarrow (\mathbf{x}'',t'')$, etc. If the arguments are omitted, the corresponding primes are retained (i.e., $\mathbf{u}(\mathbf{x}'',t'') = \mathbf{u}(2) = \mathbf{u}''$) unless confusion can arise or if only a symbolic representation is intended. The initial and boundary conditions are written simply as Φ, so the solution $T(\mathbf{x},t)$, which was written out above in detail, is simply $T = \int G(01)\Phi(1)\,d1$. Both T and G are random functions as a result of the random coefficient $\mathbf{u}(\mathbf{x},t)$. The random fluctuations in Φ and G will be denoted by ϕ and g.

The temperature-field equation can be used to formulate expressions for statistical moments of T or G. Unfortunately, each equation contains a higher-order moment because of the random coefficient $\mathbf{u}$, and an infinite set of unclosed equations or an infinite iteration expansion results. The task of devising an approximation to form a determinate mathematical problem by suitably truncating or consolidating the set of equations or the expansion is called the closure problem.

The methods of closure described below will not be restricted to steady isotropic turbulence with uniform $\nabla\langle T \rangle$ until Section (2c) where κ^t is discussed

and where the equations are reduced to the isotropic case. In order to define κ^t suitably, it will be necessary to assume that the smallest dimensions of the region $\mathcal{R}$ is large compared to the scale of turbulence λ,* so that, over the region where we wish to calculate κ^t, $\nabla\langle T\rangle$ is effectively uniform.

The Green's function for the case of zero turbulence is written with a superscript zero (since it is a zeroth approximation of G) and is not a stochastic quantity. G^0 is used below in iteration expansions. For the isotropic case G^0 is the Green's function for heat conduction in an infinite region

$$G^0(\mathbf{x},t\,|\,\mathbf{x}',t') = [4\pi\kappa(t-t')]^{-3/2}\exp\{-|\mathbf{x}-\mathbf{x}'|^2/4\kappa(t-t')\},\ t>t'.$$

a. The maximal randomness condition (MRC)

The analog of Kraichnan's MRC† for the convection problem is that the statistical dependence between $\mathbf{u}$ and T (or G) is induced solely by the random coefficient $\mathbf{u}$ and not at all by the boundary or initial conditions. It is sufficient to require that $\mathbf{u}$ and ϕ be uncorrelated to all orders of $\mathbf{u}$. If $\mathbf{u}$ and ϕ were correlated,‡ then a statistical dependence between ϕ and G would be developed through $\mathbf{u}$. The MRC prevents the transmission of any statistical information of ϕ to G. Hence the Green's function problem can be solved independently of the temperature-field problem. We have, then,

$$\langle T\rangle = \int\langle G(01)\rangle\langle\Phi(1)\rangle\ d1$$

$$\langle \mathbf{u}T\rangle = \int\langle \mathbf{u}G(01)\rangle\langle\Phi(1)\rangle\ d1$$

$$\langle T^2\rangle = \iint\langle G(01)G(02)\rangle\langle\Phi(1)\,\Phi(2)\rangle\ d1d2.$$

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*In isotropic turbulence define the scale λ to be $\lambda=\int_0^\infty f(r,o)dr$ where $f(r,t)$ is the longitudinal space-time double velocity correlation coefficient.

†The MRC was originally defined for the Fourier representation of the velocity field in homogeneous turbulence.[1] The initial conditions must be "maximally random"; i.e., the velocity field initially is independent, multivariate Gaussian (which follows from central-limit reasoning). A more formal statement of the MRC and its use to develop a hierarchy of equations for single-time moments is given by Orszag.[6,7]

‡This would be the case if, for example, part of the boundary $\mathcal{B}$ were an imaginary surface within the fluid where there were both velocity and temperature fluctuations. This condition could arise for heat transfer to an open system in which we introduce an imaginary boundary to restrict the region for numerical computation. The MRC can be satisfied by the trivial case $\phi=0$ (i.e., $T_0=\langle T_0\rangle$ and $T_B=\langle T_B\rangle$).

Thus the closure problem for the temperature field is equivalent to the closure problem for the Green's function if the MRC is specified. We will refer to the problem of calculating these temperature-field moments as the T-problem when the closure approximations are applied directly to the temperature-field and as the G-problem when the approximations are applied to the Green's function.

In the present problem the MRC need not be explicitly stated since for large times and far from the boundaries $\langle \mathbf{u}\theta(1)\rangle$, etc., $\to 0$. We also require that the velocity field be statistically homogeneous in space and time and that $\lambda^3 \int_V d^3x$.

b. Closures for T and G

In this section we describe the closures to be compared. The approximations used here are the first-iteration approximation (FIA), the third-cumulant discard (3CD), and the direct-interaction approximation (DIA). The idea of these closures is to separate the statistics of the velocity and temperature fields, so that given $\langle \mathbf{u}\mathbf{u}'\rangle$, for example, we can calculate $\langle T\rangle$, $\langle \mathbf{u}T\rangle$, and $\langle T^2\rangle$. These closures are of low enough order that $\langle \mathbf{u}\mathbf{u}'\rangle$ is sufficient information.* Note that $\langle \mathbf{u}\mathbf{u}'\rangle$ is an incomplete and non-unique statistical specification of the velocity field. Since FIA and 3CD use no variational principle or other maximizing device in relating higher to lower moments (only a statistical hypothesis on the relation between moments) the higher order statistics of the velocity field do not affect the temperature field. Although the DIA is based on a dynamical rather than a purely statistical hypothesis and includes no ad hoc assumption about the relation between moments, it too results in a temperature field that is independent of higher order velocity moments.

The FIA and 3CD specify the form of the triple moments containing θ or g as random variables. If the moment is linear in θ or g, as in the approximation for $\langle \mathbf{u}\theta\rangle$, then the closures for the T-problem are identical to those for the G-problem. The reason is that Φ appears linearly in the G-problem, so ϕ averages out. However, if the moment is bilinear in θ or g, as in the approximation for $\langle \theta^2\rangle$, the closures for the T-problem are not the same as those for the G-problem. Since Φ appears bilinearly in the G-problem, moments of the form $\langle \phi\phi'\rangle$ appear that do not arise the T-problem. The reason that the T and G problems are not identical is because T has stochastic properties Φ initially and on the boundary, whereas G does not. Therefore, specification of the form of triple moments involving g is statistically less restrictive than specification of moments

*This selection of closure approximations is chosen to parallel that of Kraichnan[8] in a discussion of the asymptotic short and long-time behaviors of random convection in homogeneous turbulence for large Péclét number.

involving θ. In other words, θ-moments are intimately tied up with statistical properties of Φ near the boundaries of R_Φ ($t_0 \leq t < \infty$), whereas g-moments are not. The exception to this case, as noted above, is when θ or g appears linearly, and the two problems are thus equivalent. In the present problem, for large times and far from the boundaries, terms involving $\langle \phi\phi' \rangle$ go to zero, so that the results from the T and G problems are identical.

The invariance and realizability properties of these closure approximations have been remarked on by Kraichnan in a different context.[8] They will not be repeated or extended to the more general case described here.

(1) The FIA. This approximation is equivalent to expanding the temperature-field in powers of Péclét number and retaining only the first order term, which corresponds to a simple perturbation expansion. The temperature fluctuations are expanded about the zeroth order fluctuations by iterating

$$\theta = \theta^0 + \int G^0(01) \nabla' \cdot [\langle \mathbf{u}'\theta' \rangle - \mathbf{u}'\theta' - \mathbf{u}' \langle T' \rangle] \, d1$$

and retaining only first order terms. A similar procedure is used for g. An alternative approach is to use the following statistical postulate for calculating $\langle \mathbf{u}\theta \rangle$ from the above equation: $\langle \mathbf{u}\mathbf{u}'\theta' \rangle = \langle \mathbf{u}\mathbf{u}' \rangle (T'^0 - \langle T' \rangle)$, where T^0 is calculated from G^0 and Φ. Equivalently, $\langle \mathbf{u}\mathbf{u}' g(12) \rangle = \langle \mathbf{u}\mathbf{u}' \rangle (G^0(12) - \langle G(12) \rangle)$. The result for $\langle \mathbf{u}\theta \rangle$ in either case is

$$\langle \mathbf{u}\theta \rangle = - \int G^0(01) \langle \mathbf{u}\mathbf{u}' \rangle \cdot \nabla' T'^0 \, d1.$$

For calculating $\langle \theta^2 \rangle$ the needed FIA postulate for the T-problem is $\langle \mathbf{u}'\theta'\theta \rangle = \langle \mathbf{u}'\theta \rangle (T'^0 - \langle T' \rangle)$ where $\langle \mathbf{u}'\theta \rangle$ is also evaluated with the FIA. The result is

$$\langle \theta^2 \rangle = \iint G^0(01) G^0(02) \langle \mathbf{u}''\mathbf{u}' \rangle : \nabla' T'^0 \nabla'' T''^0 \, d1 \, d2.$$

The corresponding G-problem postulate is $\langle \mathbf{u}''' g(01) g(32) \rangle = \langle \mathbf{u}''' g(01) \rangle (G^0(32) - \langle G(32) \rangle)$ where $\langle \mathbf{u}''' g(01) \rangle$ is also evaluated with the FIA. The following term must be added to the above result for $\langle \theta^2 \rangle$:

$$\iint\left\{\langle G(01)\rangle\langle G(02)\rangle+\iint G^0(03)G^0(04)\nabla'''\nabla^{IV}:\langle \mathbf{u}^{IV}\mathbf{u}'''\rangle G^0(32)G^0(41)\,d3d4\right\}\langle\phi(1)\phi(2)\rangle\,d1d2$$

where $\langle G\rangle$ is given by the FIA by

$$\langle G(01)\rangle = G^0(01)+\iint G^0(02)\langle \mathbf{u}'''\mathbf{u}''\rangle:\nabla''G^0(23)\nabla'''G^0(31)\,d2d3.$$

(2) The 3CD. The statistical postulate for this approximation is that all triple moments involving θ or g are zero. That is, moments of the form $\langle \mathbf{u}\mathbf{u}\theta\rangle = \langle \mathbf{u}\mathbf{u}\mathrm{g}\rangle = \langle \mathbf{u}\theta\theta\rangle = \langle \mathbf{u}\mathrm{g}\mathrm{g}\rangle = 0$ for arbitrary arguments of θ, $\mathbf{u}$, and g. The results for the T-problem are

$$\langle \mathbf{u}\theta\rangle = -\int G^0(01)\langle \mathbf{u}\mathbf{u}'\rangle\cdot\nabla'\langle T'\rangle\,d1$$

$$\langle\theta^2\rangle = \iint G^0(01)G^0(02)\langle \mathbf{u}''\mathbf{u}'\rangle:\nabla'\langle T'\rangle\nabla''\langle T''\rangle\,d1\,d2$$

The G-problem results are identical except for the additional term in $\langle\theta^2\rangle$:

$$\iint\left\{\langle G(01)\rangle\langle G(02)\rangle+\iint G^0(03)G^0(04)\nabla'''\nabla^{IV}:\langle \mathbf{u}^{IV}\mathbf{u}'''\rangle\langle G(32)\rangle\langle G(41)\rangle\,d3d4\right\}\langle\phi(1)\phi(2)\rangle\,d1d2$$

where $\langle G\rangle$ is given by

$$\langle G(01)\rangle = G^0(01)+\iint G^0(02)\langle \mathbf{u}'''\mathbf{u}''\rangle:\nabla''G^0(23)\nabla'''\langle G(31)\rangle\,d2d3.$$

(3) The DIA. This approximation has been discussed in detail by Kraichnan.[1,2,3] No explicit statistical postulate is made about the relations between moments, contrary to the FIA and 3CD, because the approximation concerns the dynamics of the random convection rather than the form of a particular statistical moment. From Equation 7.3 of Reference (3) the DIA result for $\langle \mathbf{u}\theta\rangle$ is

$$\langle \mathbf{u}\theta\rangle = -\int\langle G(01)\rangle\langle \mathbf{u}\mathbf{u}'\rangle\cdot\nabla'\langle T'\rangle\,d1$$

where $\langle G \rangle$ is given by

$$\langle G(01) \rangle = G^0(01) + \iint G^0(02) \langle \mathbf{u}''' \mathbf{u}'' \rangle : \nabla'' \langle G(23) \rangle \nabla''' \langle G(31) \rangle d2d3.$$

The calculation of $\langle \theta^2 \rangle$ is much more difficult than for the FIA and 3CD, and we have not succeeded in developing a closed expression for it. Given $\langle G \rangle$, $\langle \mathbf{uu}' \rangle$, and $\langle T \rangle$, however, one can calculate $\langle \theta\theta' \rangle$ from the following generalization of Equation 11.33 of Reference (2):

$$\mathcal{L} \langle \theta\theta' \rangle = \nabla \langle T \rangle \cdot \int \langle G(12) \rangle \langle \mathbf{uu}'' \rangle \cdot \nabla'' \langle T'' \rangle d2 + \nabla \cdot \int \langle \mathbf{uu}'' \rangle \cdot$$

$$\left[\langle G(12) \rangle \nabla'' \langle \theta\theta'' \rangle + \langle G(02) \rangle \nabla'' \langle \theta'\theta'' \rangle \right] d2.$$

Then $\langle \theta^2 \rangle$ can be recovered by taking $(\mathbf{x}', t') \Rightarrow (\mathbf{x}, t)$. Because of the difficulty of this problem, the comparison of $\langle \theta^2 \rangle$ for the various approximations will not be discussed. This means, unfortunately, that we will be unable to discuss the correlation coefficient

$$\psi \equiv \langle \mathbf{u}\theta \rangle \left[\frac{1}{3} \langle \mathbf{u} \cdot \mathbf{u} \rangle \langle \theta^2 \rangle \right]^{-1/2}.$$

c. Specialization to the present problem.

Now we introduce the conditions of the present problem. Assume a stationary, homogeneous turbulence with $\langle \mathbf{U} \rangle = 0$. Two parallel planes within this field are separated by $L >> \lambda$ and are each maintained at a different uniform temperature such that the MRC is satisfied (e.g., $\theta_B \equiv 0$). Then for steady state ($t \to \infty$) and far from the boundaries we expect on physical grounds that a uniform $\nabla \langle T \rangle$ will develop, $\nabla \langle T \rangle = \mathbf{A}$. This, we hope, leads to the existence of an eddy diffusivity κ^t independent of $\mathbf{A}$. The result for $\langle \mathbf{u}\theta \rangle$ given by the FIA includes the factor $\nabla T^0 \equiv \mathbf{A}^0$. The relation between $\mathbf{A}$ and $\mathbf{A}^0$ consistent with the FIA is

$$\mathbf{A} = \boldsymbol{\alpha} \cdot \mathbf{A}^0$$

where $\boldsymbol{\alpha} = 1 + \iint \nabla G^0(01) \langle \mathbf{u}'' \mathbf{u}' \rangle \cdot \nabla' G^0(12) d1d2$. For isotropic turbulence $\boldsymbol{\alpha}$ is defined by one scalar α, so $\mathbf{A} = \alpha \mathbf{A}^0$. Let us define

$$\kappa_0 = \int G^0(01)\langle \mathbf{u}\mathbf{u}' \rangle \, d1.$$

Then the FIA result is $\kappa^t_{FIA} = \kappa_0/\alpha$, and the 3CD result is simply $\kappa^t_{3CD} = \kappa_0$. Note that $\langle G \rangle$ is not needed for the 3CD or FIA results. The DIA result is

$$\kappa^t_{DIA} = \int \langle G(01) \rangle \langle \mathbf{u}\mathbf{u}' \rangle \, d1$$

where the equation for $\langle G \rangle$ may be rewritten as the solution of

$$\mathcal{L}\langle G(01) \rangle = \int \langle \mathbf{u}''\mathbf{u} \rangle : \nabla \langle G(02) \rangle \nabla'' \langle G(21) \rangle \, d2 \equiv H(01)$$

which is the form we shall use for numerical calculation.

For the case of steady, homogeneous, incompressible, isotropic turbulence, $\langle G \rangle$ reduces to the special form $\langle G(\mathbf{x}, t \mid \mathbf{x}', t') \rangle = \langle G(|\mathbf{x}-\mathbf{x}'|, t-t') \rangle$ and similarly for G^0.* The velocity covariance reduces to the form

$$\langle \mathbf{u}(\mathbf{x}, t)\, \mathbf{u}(\mathbf{x}', t') \rangle = \mathbf{Q}(\mathbf{x}-\mathbf{x}', t-t')$$

where

$$\mathbf{Q}(\mathbf{r}, t) = |u|^2 \hat{\mathbf{r}}\hat{\mathbf{r}} - \left[\frac{r}{2}\frac{\partial f}{\partial r}(r, t)\right] + |u|^2 \mathbf{1}\left[f(r, t) + \frac{r}{2}\frac{\partial f}{\partial r}(r, t)\right].$$

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*This is only true when $\langle G \rangle$ or G^0 is multiplied by $\langle \mathbf{u}\mathbf{u}' \rangle$ with the same arguments, so that far from the boundaries the spherical approximation is good over distances the order of λ. (Keep in mind that $\langle G \rangle$ and G^0 are zero on $\mathcal{B}$.) The spherical approximation cannot be used in determining α for the FIA, since in the integral expression for α there is one G^0 not weighted by $\langle \mathbf{u}\mathbf{u}' \rangle$ with corresponding arguments. In that case we must use the nonhomogeneous G^0 for parallel planes separated by $L \gg \lambda$. Let $\mathbf{e}_1$ be the direction normal to the planes with coordinate x, $r = |(\mathbf{x}-\mathbf{x}') \times \mathbf{e}_1|$, and $t > t'$. Then G^0 takes the form

$$G^0(x, x', r, t-t') = \frac{1}{\pi L}\sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{n\pi x'}{L}\right)\int_0^{\infty} d\xi \xi J_0(\xi r) \exp\left\{-\kappa\left[\xi^2 + \left(\frac{n\pi}{L}\right)^2\right](t-t')\right\}.$$

In this equation $|u|^2 = 1/3 \langle \mathbf{u} \cdot \mathbf{u} \rangle$, $r = |\mathbf{r}|$, $\hat{\mathbf{r}} = \mathbf{r}/r$, and f is the longitudinal space-time velocity correlation coefficient. The eddy diffusivity goes to the diagonal form $\kappa^t = 1\,\kappa^t$. For large times ($t \to \infty$) κ^t may be written

$$\kappa^t = 4\pi |u|^2 \int_0^\infty dt \int_0^\infty r^2\, dr\, G(r,t) \left[f(r,t) + \frac{r}{3} \frac{\partial f}{\partial r}(r,t) \right]$$

where $G(r,t) = G^0(r,t)/\alpha$ for the FIA, $G(r,t) = G^0(r,t)$ for the 3CD, and $G(r,t) = \langle G(r,t) \rangle$ for the DIA. Here α will depend on position and the separation distance L, indicating that the FIA is not a local enough approximation to given uniform κ^t. $\langle G(r,t) \rangle$ for the DIA is the solution of

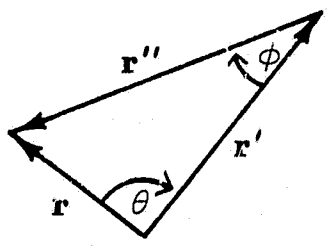
$$\left\{ \frac{\partial}{\partial t} - \kappa \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \right\} \langle G(r,t) \rangle = H(r,t) \qquad (1)$$

where $\langle G(r,0) \rangle = \delta(r)/2\pi r^2$, $\langle G(r,t) \rangle \xrightarrow[r \to \infty]{} 0$, and H is given by

$$H(r,t) = |u|^2 \int_0^t dt' \int_0^\infty 2\pi r'^2\, dr' \int_{-1}^1 d\mu \langle G(r',t') \rangle \left\{ \left[f(r',t') + \frac{\gamma^2 r'}{2} \frac{\partial}{\partial r'} f(r',t') \right] \times \right.$$

$$\left. \frac{\partial^2}{\partial r''^2} \langle G(r'',t'') \rangle + \frac{2}{r''} \left[f(r',t') + \left(1 - \frac{\gamma^2}{2} \right) r' \frac{\partial f}{\partial r'}(r',t') \right] \frac{\partial}{\partial r''} G(r'',t'') \rangle \right\}$$

where $\gamma^2 = (1 - \mu^2) r^2 / r''^2$, $r''^2 = r^2 + r'^2 - 2\mu r r'$, $t'' = t - t'$, and use has been made of spatial homogeneity. The geometry of the space convolution is shown in the following figure.



$$\mathbf{r}'' = \mathbf{r} - \mathbf{r}'$$

$$\mu = \cos\theta$$

$$\gamma = \sin\phi$$

d. Input information.

The calculation of κ^t requires specification of κ, $|u|$, and $f(r,t)$. Data are available for $f(r,t)$ for the case of nearly isotropic grid-generated turbulence and are summarized by Favre.[9] The behavior of f is too complex to permit efficient calculation of H, so for the present work simplified approximations will be used. One simple model that was briefly considered is the "on-off" function

$$f_1(r\ t) = \begin{cases} 1, & r < \lambda \text{ and } t < \tau \\ 0 & r > \lambda \text{ or } t > \tau \end{cases}$$

where λ and τ are the integral length and time scales. Unfortunately, f_1 is not realizable because the corresponding energy spectrum function

$$\tilde{E}(k) = \frac{3|u|^2\lambda}{\pi} \left\{ \frac{\sin k\lambda}{k\lambda} \left[1 - \frac{1}{3}(k\lambda)^2 \right] - \cos k\lambda \right\}$$

is not positive for all k. Another model is the exponential function $f_2(r,t) = \exp\{-r/\lambda - t/\tau\}$, which has an undefined Taylor microscale. More complex and realistic models can be introduced if the numerical procedures prove feasible.

3. NUMERICAL CALCULATION OF $\langle G \rangle$

One can now calculate κ^t for the FIA and 3CD since G^0 and $f(r,t)$ are given (and α can be evaluated from these). However, the DIA result for κ^t involves $\langle G \rangle$, which was given above by the implicit equation $\mathcal{L}\langle G \rangle = H$ where H is a nonlinear functional of $\langle G \rangle$. This equation, Equation (1), must be solved by numerical approximation.

We follow the usual method of approximating $\langle G \rangle$ on a space-time mesh as the solution of a set of difference equations which are solved by proceeding from one time layer to the next.* The set is consistent with Equation (1) as the space-time mesh is allowed to become arbitrarily dense. Unfortunately, little more

*The numerical solution of parabolic partial differential equations is discussed in (10), (11, Ch. 7), (12, Ch. 8), (13, Ch. 2), and (14), in which many references to the literature may be found.

can be said about the validity of the approximation. The existence of a unique solution to Equation (1) has not been demonstrated, nor have the stability and convergence of numerical schemes been investigated. These schemes, similar to those for solution of the spherical heat equation with a source, would be known to be stable and convergent if H and initial $\langle G \rangle$ were bounded (or else if certain derivatives of $\langle G \rangle$ have singularities of sufficiently low order as $t \to 0$), which is not the case. Also, it is difficult to reproduce numerically the strong initial singularity in $\langle G \rangle$, and hence an infinitesimal-discretization-error analysis may not be appropriate for approximations to Equation (1). Nevertheless, we will consider a posteriori evidence of convergence and stability plus the consistency requirement to be sufficient justification for the suitability of a numerical method.

It is convenient to dimensionally normalize both the difference and differential equations. The length scale is λ, so then normalized $\langle G \rangle$ is $\lambda^3 \langle G \rangle$ and normalized r is r/λ . If t is normalized by viscous decay time, i.e., as $t\nu/\lambda^2$, then in Equation (1) we take $\kappa \to$ (Prandtl No.)$^{-1}$ and $|u| \to$ Reynolds No. ($|u| \lambda/\nu$). If t is normalized by conduction time, i.e., as $t\kappa/\lambda^2$, then $\kappa \to 1$ and $|u| \to$ Péclét No. ($|u|\lambda/\kappa$). Or finally, if t is normalized by eddy circulation time, i.e., as $t|u|/\lambda$, then $\kappa \to$ (Péclét No.)$^{-1}$ and $|u| \to 1$. We leave the choice of time scale arbitrary.

a. Difference equations for $\langle G \rangle$

The solution $\langle G(r_n, t_m) \rangle$ of Equation (1) is to be approximated by G_n^m (or simply **G**) for all points (n,m) on the space-time mesh. We take uniform space increments h so that $r_n = nh$: $n = 0, 1, 2, \ldots N$. The range of r is finite with $r_N \gg \lambda$ such that integrals with respect to r can be truncated at r_N with error $O(h^2)$. The time increments are arbitrary, $\ell_m = t_m - t_{m-1}$: $m = 1, 2, \ldots M$ where $\ell_0 = 0$. The assignment of ℓ_m suggested by Douglas[10] is $\ell_{m+1} / \ell_m =$ constant $b \geq 1$ $(m > 0)$ which takes into account the expected increase in smoothness of $\langle G \rangle$ with respect to r as time progresses. The time increments may also be written $\ell_{m+1} = \ell_1 + (1-b) \sum_{k=1}^{m} \ell_k$ or $\ell_{m+1} = b^m \ell_1$ for $m > 0$.

Here we list some definitions of difference operations on space functions ϕ and time functions ψ:

Laplacian (spherical) central difference:

$$\delta_n^2 \phi_n = \begin{cases} (1/h^2) \left[\left(1 - \frac{1}{n}\right) \phi_{n-1} - 2\phi_n + \left(1 + \frac{1}{n}\right) \phi_{n+1} \right], & n > 0 \\ (6/h^2) \left[\phi_1 - \phi_0\right], & n = 0 \end{cases}$$

Gradient central difference:

$$\delta_n \phi_n = \begin{cases} (1/2h)\ [\phi_{n+1} - \phi_{n-1}] \quad , & n > 0 \\ (1/2h)\ [4\phi_1 - \phi_2 - 3\phi_0] , & n = 0 \end{cases}$$

Spatial interpolation:

$$\phi_x = \xi\, \phi_n + (1 - \xi)\, \phi_{n+1}, \quad (n = \mathrm{mod}\,(x),\ \xi = x - n)$$

Two-layer average:

$$^{(2)}\tilde{\psi}^{m+\theta} = \theta\, \psi^{m+1} + (1 - \theta)\, \psi^m, \quad (0 \le \theta \le 1,\ t_{m+\theta} = t_m + \theta \ell_{m+1})$$

Three-layer average:

$$^{(3)}\tilde{\psi}^m = \frac{1}{3}\,(\ell_m/\bar{\ell}_m)\, \psi^{m+1} + \frac{1}{3}\,\psi^m + \frac{1}{3}\,(\ell_{m+1}/\bar{\ell}_m)\, \psi^{m-1}, \quad \left(\bar{\ell}_m = \frac{1}{2}\,[\ell_m + \ell_{m+1}]\right)$$

Two-layer time-difference:

$$\Delta_t^{(2)}\, \psi^{m+\theta} = [\psi^{m+1} - \psi^m]/\ell_{m+1}$$

Three-layer time-difference:

$$\Delta_t^{(3)}\, \psi^m = [(1/b)\, \psi^{m+1} + (b - 1/b)\, \psi^m - b\psi^{m-1}]/2\bar{\ell}_m .$$

The errors associated with applying these approximations (see Appendix) are all second order with respect to mesh spacing if $\theta = 1/2$. If $\theta \neq 1/2$ then the two-layer time difference has a first order truncation error.

The quadrature formula for H is based on the trapezoidal rule. Similar formulae may be obtained for Simpson's rule, but the error terms will involve higher order derivatives. The integrand of H, except for the factor $2\pi r'^2$, is discretized by approximation of the derivative terms to obtain $P(r_n, r_{n'}, \mu_j, t_m, t_{m'} \mid \mathbf{G})$ defined by

$$P(\cdots|G) = G_{n'}^{m'} \left\{F_1 \left[\underset{\sim}{\delta}_x^2 \underset{\sim}{G}_x^{m-m'}\right] + F_2 \left[\underset{\sim}{\delta}_x \underset{\sim}{G}_x^{m-m'}\right]\right\}, \quad (x^2 = n^2 + n'^2 - 2nn'\mu_j)$$

where

$$F_1 = |u|^2 \left\{f(r_{n'}, t_{m'}) + \frac{\gamma^2 r_{n'}}{2}\left[\frac{\partial}{\partial r_{n'}} f(r_{n'}, t_{m'})\right]\right\}$$

$$F_2 = |u|^2 \left\{\frac{2 r_{n'}}{r_x}(1-\gamma^2)\left[\frac{\partial}{\partial r_{n'}} f(r_{n'}, t_{m'})\right]\right\}.$$

The integration over r' is performed by a modified trapezoidal rule obtained by integrating the first order Lagrangian interpolation polynomial times the factor $2\pi r'^2$ over each interval such that

$$\int_0^{r_N} 2\pi r'^2 \psi(r')\,dr' \approx \frac{\pi h^3}{12}\psi_0 + \pi h^3\left(N^2 - \frac{1}{3}N + \frac{1}{12}\right)\psi_N + \sum_{n=1}^{N-1} 2\pi h^3\left(n^2 + \frac{1}{6}\right)\psi_n.$$

The μ-integration is over intervals $(\Delta\mu) = 2/J$,

$$\int_{-1}^{1} \psi(\mu)\,d\mu \approx (\psi_0 + \psi_J)/J + \frac{2}{J}\sum_{j=1}^{J-1}\psi_j.$$

Since the time intervals increase monotonically, it is desirable to perform the time convolution by summing simultaneously from times 0 and t_m to $1/2\ t_m \equiv t_{m_2}$ where $m_2 = \log_b [1/2(1 + b^m)]$.* The indicated integration is

$$\int_0^{t_m} \psi(t')\,dt' \approx \frac{1}{2}[\ell_1 \psi_0 + 2\ell_{m_2}\psi_{m_2} + \ell_1 \psi_m] + \sum_{m'=1}^{m_2-1} \bar{\ell}_{m'}(\psi_{m'} + \psi_{m-m'}).$$

The triple sum will be denoted by $\Sigma_{n'jm'}^{nm}$. Then the right hand side of Equation (1) is approximated by

*Since m_2 is not generally an integer, a small correction for the interval $(m_2 - 1, m_2 + 1)$ must be made in practice.

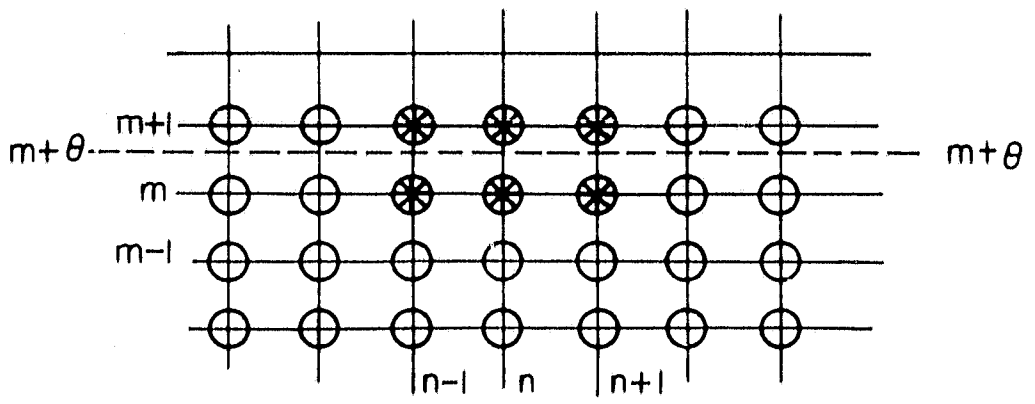
$$H_n^m = \sum_{n'\,jm'}^{nm} P(r_n,\ r_{n'},\ \mu_j,\ t_m,\ t_{m'}\ |G)$$

which has a truncation error maintained at $O(h^2) + O(\ell_m^2)$ with the restrictions outlined in the Appendix. Unfortunately, even if we succeed in restricting the truncation error to this order, the overall discretization error may not be small since it obeys a nonlinear integral equation involving $\langle G \rangle$.

We consider two types of difference equations for **G**. (I) The Crank-Nicolson form, which is set up by approximating Equation (1) on the fictitious time layer $m + \theta$, $0 \leq \theta \leq 1$, gives an implicit equation for values of **G** on time layer $m + 1$:

$$\Delta_t^{(2)} G_n^{m+\theta} - \kappa\, \delta_n^2\, {}^{(2)}\tilde{G}_n^{m+\theta} = \tilde{H}_n^{m+\theta}. \qquad (2)$$

The truncation error associated with (2) is $O(h^2) + O(\ell_{m+1})$ unless $\theta = 1/2$, for which it is $O(h^2) + O(\ell_{m+1}^2)$. The latter case is preferred unless stability considerations require $\theta > 1/2$.* The mesh points of **G** appearing in (2) are shown schematically in the following figure: those associated with $\mathfrak{L}$ are marked as an asterisk, and those associated with H are circled. The time increments are shown to be uniform for simplicity.

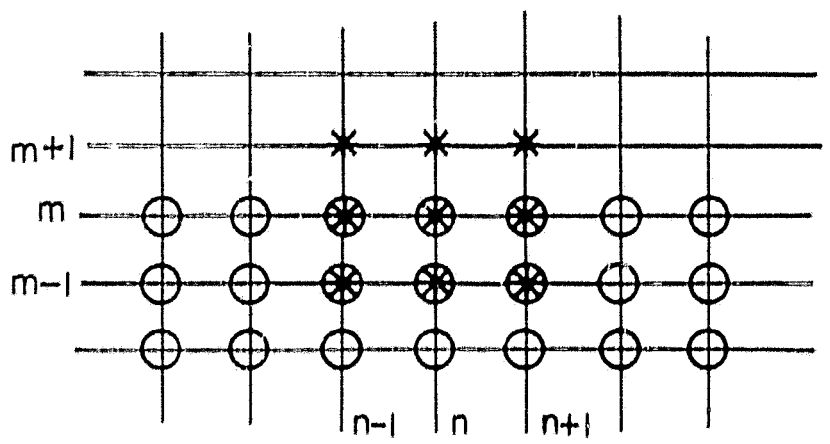


(II) The multilayer form is obtained by applying the discretized heat operator to three adjacent time layers,

$$\Delta_t^{(3)} G_n^m - \kappa\, \delta_n^2\, {}^{(3)}\tilde{G}_n^m = H_n^m. \qquad (3)$$

*If H =0 (no turbulence) Equation (2) is stable and convergent for $\theta \geq 1/2$.

The truncation error in this case is $O(h^2) + O([\ell_m^*]^2)$, $\ell_m^* = (\ell_m \ell_{m+1})^{1/2}$. The mesh points for Equation (3) are laid out below.



b. Solution of the difference equations.

Let g be the vector of values of G for all n on the (m+1) time layer. We wish to solve (2) and (3) for g in terms of G for all previous time layers.

Equations (2) and (3) may be written as

$$\mathbf{B}\mathbf{g} = \mathbf{d} + \mathbf{z}\{\mathbf{g}\} \tag{4}$$

where the left side represents the discretized part of $\mathcal{L}\langle G\rangle$ on time layer (m+1), the vector d comes from the contributions to $\mathcal{L}\langle G\rangle$ and H of all time layers $\leq m$, and the vector functional z is from the portion of H depending on the (m+1) time layer. The matrix B is tri-diagonal and may be inverted directly by the Thomas algorithm.*

If (4) is of the Crank-Nicolson form, the term z is treated as a perturbation. A sequence of iterations is set up with the k^{th} iterate $\mathbf{g}^{(k)}$ given by

$$\mathbf{g}^{(k)} = \omega \mathbf{B}^{-1}\left(\mathbf{d} + \mathbf{z}\left\{\mathbf{g}^{(k-1)}\right\}\right) + (1-\omega)\,\mathbf{g}^{(k-1)}$$

where ω is a constant called the relaxation factor. For $\omega > 1$ this is the method of successive overrelaxation. The zeroth interate is calculated from (4) with the

*The Thomas algorithm[11, p. 341] is a normalized form of Gaussian elimination (see Appendix). It is stable with respect to round-off errors if B is tri-diagonal and diagonally dominant, as it is for Equations (2) and (3).

argument $g = G^{m+1}$ of z replaced by G^m. The iteration is continued until the parameter $\{\max_n ||g^{(k)}| - |g^{(k-1)}||/\max_n |g^{(k)}|\}$ is arbitrarily small, usually 10^{-4}.

If (4) is of the multilayer form, then $z = 0$ and (4) is solved directly. Equation (3), however, applies to three adjacent time layers, and so Equation (2) must be used to calculate G^1.

The outer boundary condition for G is that $G_N^m = 0^*$ for all m. The values of G for $n = 0$, the inner boundary, are given by (2) or (3). An alternative and simpler scheme for G_0^m would be to take $\delta_0 G_0^m = 0$.

The initial condition of $\langle G \rangle$ is supposed to be the spherical Dirac delta-function. The numerical approximation is to take G_n^0 to be a spherical Gaussian with initial variance $\sigma_0^2 \ll \lambda^2$. This is only possible if σ_0 is the same order as h, and so we expect a large interaction between σ_0 and the truncation error. A good approximation to $\langle G \rangle$ can be recovered only by taking $\sigma_0 \to 0$ where $h \to 0$ faster. The practicality of this procedure is still doubtful.

c. Numerical difficulties.

The numerical approximation of $\langle G \rangle$ is subject to the usual difficulties experienced with parabolic systems regarding the effect of mesh size on convergence and stability. In addition, the singularity of the initial condition and the nonlinear convolution make error and stability analyses difficult (although energy methods may be useful). Small truncation error does not guarantee a small total discretization error, even for a stable numerical scheme. Below we list details of some expected numerical difficulties associated with the singular nature of G_n^0.

(1) The truncation errors for (2) and (3) have terms $O(h^2)$ if the coefficients of those terms, which involve $\nabla^4 \langle G \rangle$, are uniformly bounded. The biharmonic operator appears in the lowest truncation terms from δ_n^2 and the trapezoidal r′-sum. If Simpson's rule for the r′-integration were used, there would be sixth-order derivatives in the lowest terms. The sharpness of the initial condition makes it difficult to maintain small truncation errors unless $h \ll \sigma_0$ and ℓ_1 be chosen sufficiently small to strongly overdamp these errors.

(2) Besides having an essential singularity at zero time, $\langle G \rangle$ has sharp and nearly discontinuous behavior that persists for slightly longer times, so that

*We actually require $G_{n>N}^m = 0$. These terms appear in H as formulated for the infinite domain and hopefully make a negligible contribution for large enought r_N.

nearly-unbounded derivatives are not restricted to $t = 0$. The Fourier transform of $\langle G \rangle$ for times $t \ll \lambda'/|u|$ is identical to the large Péclét number result of Lee[15, ff. Equation (29)] for wavenumbers in the equilibrium subrange. Instead of falling off monotonically with increasing r, $\langle G \rangle$ rises to a cusp at $r = 2|u|t$ which becomes an infinitely sharp-cut-off when $\kappa = 0$:*

$$\lim_{\kappa \to 0} \langle G(r, t) \rangle = \left\{ \begin{array}{ll} [2\pi |u| t]^{-2} (4|u|^2 t^2 - r^2)^{-1/2}, & r < 2|u| t \\ 0, & r > 2|u| t \end{array} \right\} t \ll \lambda' |u|.$$

(3) The severity of the discretization error is sometimes illustrated by the appearance of large oscillations associated with the truncation of high order derivatives. Lack of oscillations does not imply convergence, but the appearance of large ones indicates that the discretization error is also large. In order to gain some insight into this behavior, consider the Crank-Nicolson case with uniform time increments. We assume that the nonhomogeneous part of Equation (1) can be expanded as $\ell H_n^m = \Sigma_j S_m^j X_n^j$ and that **G** itself can be expanded as $G_n^m = \Sigma_j T_m^j X_n^j$ over eigenvalues λ_j of the equation $(A - I\lambda_j) X^j = 0$ where A is the matrix derived from the heat operator (with $X_N = 0$)

$$A \begin{bmatrix} 6 & -6 & & & & \\ 0 & 2 & -2 & & & 0 \\ & -1\ 2 & 2 & -3\ 2 & & \\ & & -\left(1 - \frac{1}{n}\right) & 2 & -\left(1 + \frac{1}{n}\right) & \\ & 0 & & -\left(1 - \frac{1}{N-1}\right) & & 2 \end{bmatrix}$$

and the X's correspond to the space-part of the separable solution to the heat equation. The problem is to determine the properties of T_m^j affecting stability

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*This behavior of $\langle G \rangle$ was discussed by Roberts[16], who obtained the zero-κ formula, and by Kraichnan[8]. The form of $\langle G \rangle$ for $\kappa \neq 0$ corresponding to Roberts' result has not been reduced beyond the integral forms $\langle G(r,t) \rangle = (2\pi^2 r|u|t)^{-1} \int_0^\infty dk \sin(kr) J_1(2|u|kt) \exp\{-\kappa k^2 t\}$ corresponding to direct inversion of Lee's result, or

$\langle G(r, t) \rangle =$

$$[(4\pi r)(2|u|\pi t)^2 \sqrt{\pi\kappa t}]^{-1} \int_0^{(2|u|t)^2} d\zeta \, [(2|u|t)^2 - \zeta]^{-1/4} \exp\{-\zeta/4\kappa t\} \sinh\{r\sqrt{\zeta}\, 2\kappa t\}$$

from a convolution theorem.

and oscillatory behavior. Straightforward substitution of these definitions into Equation (2) yields

$$T_m^j = \sum_{m'=0}^{m} (\alpha^j)^{m-m'} Y_{m'}^j,$$

where

$$Y_0^j = a^j,\ Y_{m>0}^j = {}^{(2)}\tilde{S}_{m+\theta}^j/(1+\theta\lambda_j\rho),\ \alpha^j = 1 - \lambda_j\rho/(1+\theta\lambda_j\rho),\ \rho = \kappa\ell/h^2,$$

and a^j are the coefficients defined by the initial condition

$$a^j = \sum_{n=0}^{N-1} \ell_n G_n^0 X_n^j$$

where ℓ_n are the weighting factors

$$\sum_{n=0}^{N-1} \ell_n X_n^j X_n^k = \delta^{jk}.$$

Crandall[17] investigated the homogeneous system ($H = 0$) for which $T_m^j = a^j(\alpha^j)^m$. For this special case stability obtains if $|\alpha| < 1$, and no oscillatory modes appear if $\alpha > 0$; for given ρ, stable and non-oscillatory response obtains if $\theta > 1 - 1/\rho\,\|\lambda\|_\infty$, whereas mere stability requires $\theta > 1/2 - 1/\rho\,\|\lambda\|_\infty$.* The nonhomogeneous system treated here is far more complicated. The S's are functionals of all the T's and X's, and so T obeys a nonlinear functional equation with perhaps no uniform criteria for stability or suppression of oscillations. This analysis should be extended further and be applied to the multilayer and variable-ℓ forms of the difference equations.

(4) The last expected difficulty that we mention concerns the rate of convergence of the iteration sequence for the Crank-Nicolson form. Rapid convergence requires that **z** be a small fraction of the term ℓH; but since H is a time convolution, **z** is a linear functional of G_n^0 which is nearly singular. Consequently, **z** may make a significant contribution to ℓH, and large initial truncation errors may propagate directly to **g**.

*The uniform norm $\|\lambda\|_\infty = \max_j |\lambda_j|$ is called the spectral radius of A. Application of Gerschgorin's theorem yields an estimate of 17/2 as an upper bound of $\|\lambda\|_\infty$.

d. Summary of numerical work.

An incomplete and inconclusive investigation of numerical procedures for calculating G was carried out on the IBM 7040-7094 Direct-Couple System at the University of Washington Computer Center at various times during 1966 and 1967. Nearly all numerical experiments were made with the parametric values $\kappa = \lambda = r = 1$ and $h = 0.1$. The overall mesh size was (N, M, J) = (100, 200, 100) or (50, 100, 50) with nearly identical results in either case.

Before the numerical schemes described above were tried, a straightforward explicit scheme ($\theta = 0$) was tried with uniform $\ell = 0.004$ so that $\rho = 2/5$, the lower stability limit of the difference scheme used here for the heat equation. For $|u| = 0$ a strong dependence of the shape of G_n^0 on the behavior of G was found. For $|u| = 1$ the scheme was extremely unstable, so this approach was abandoned.

Next was tried the implicit scheme corresponding to Equation (2) with $\theta = 1/2, \omega = 1.3$, uniform ℓ, and Gaussian G_n^0 with $\sigma_0 = h$. Fairly extensive tests were made to determine the accuracy of the numerical methods: one result was that the triple integration was only accurate to about 5%, regardless of whether the trapezoidal or Simpson's rules were used. For $|u| = 0$ and $\ell = 0.1$ oscillations occurred with amplitudes and decay rates of the same order as for G itself; as ℓ was decreased, the amplitudes decreased until, for $\ell = 0.01$, G remained positive, and for $\ell = 0.004$, the oscillations effectively disappeared. The calculation time for $|u| \neq 0$ was found to be excessive. For example, for the larger mesh it required 3.6 minutes to step off one time layer; whereas, for a course mesh with N = J = 25, h = 0.2, $\ell = 0.02$, and $|u| = 10$, only 16 layers were calculated in 45 minutes using $f_2(r,t)$. No further experiments were made after it was found that H had been incorrectly reduced to the isotropic case for the implicit numerical method.

It was decided to extend the computer program to include the variable-ℓ and multilayer schemes before correcting H, since it was felt necessary to have small time increments initially and desirable to eliminate the iteration. The main features of these programs are described in the Appendix.

4. SUGGESTIONS FOR COMPLETING THE CALCULATION

The following suggestions may be helpful in reducing the severity of the numerical troubles.

(1) The dimensionality of the initial singularity may be too large. Lower-order delta-function initial conditions may be achieved, for example, by treating

$r\langle G(r,t)\rangle$ as the dependent variable. In this case the spherical Laplacian operator goes over to the one-dimensional Laplacian.

(2) Because the initial singularity occurs at the origin $r = 0$, it may be appropriate to use nonuniform space increments h_n^m or expanded coordinates which would be time dependent to account for the spread of $\langle G\rangle$. The numerical analysis would be considerably more complicated than for uniform h.

(3) It may be worthwhile to use the short-time analytic results for $\langle G\rangle$ to begin the calculation without spurious oscillations. The finite-difference calculation would begin at some time $t \ll \lambda/|u|$ where $\langle G\rangle$ is likely to be much smoother than it was initially.

(4) The calculation can be done much more easily in Fourier coordinates for which the initial condition of $\langle\tilde{G}(k,t)\rangle$ * is unity for all wavenumbers. The number of independent variables is the same for $\langle G\rangle$ and $\langle\tilde{G}\rangle$, and both H and $\tilde{H}$ require three integrations. In fact, Lee[15] has evaluated $\langle\tilde{G}\rangle$ for $f(r,t)$ corresponding to the energy spectrum function for the final period of decay and the asymptotic modal time correlation of Kraichnan.[1] We want, however, to be able to generalize the techniques to nonhomogeneous turbulence. For that case $\langle\tilde{G}\rangle$ is initially diagonal with respect to the two wavenumbers for the same directions of nonhomogeneity. Just as for the homogeneous case, $\langle G\rangle$ and $\langle\tilde{G}\rangle$ have the same number of independent variables; H and $\tilde{H}$ each have one time integration and the same number of integrations over coordinates or wavenumbers in directions of homogeneity. Unfortunately, for each nonhomogeneous direction, for which there is one integration in H, there are seven integrations (or sums for a finite domain) for $\tilde{H}$.† For a suitable Fourier expansion of $\langle\mathbf{uu}'\rangle$ this seven-fold integration can be reduced to a three-fold one. If this number of integrations remains intolerable, an alternative procedure would be to calculate $\langle\tilde{G}\rangle$ for small times, invert to $\langle G\rangle$, and then finish the calculation of $\langle G\rangle$ for intermediate and large times.

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*The tilde denotes a suitably-defined Fourier coefficient.

†This can be seen by examining H, written symbolically as $H = [\nabla\cdot\langle\mathbf{uu}'\rangle\langle G\rangle * [\cdot\nabla\langle G\rangle]$ where the asterisk represents space-time convolution. For each nonhomogeneous direction H produces one integration from the space convolution, one from each gradient operation, and four from the $\langle\mathbf{uu}'\rangle\langle G\rangle$ product.

APPENDIX

a. Tabulation of truncation errors

Direct application of the difference and quadrature operators in Section (3a) yields the following truncation errors:

$$\delta_n^2 \phi(r_n) - \nabla_{r_n}^2 \phi(r_n) = \frac{h^2}{12\beta} \nabla_{r_n}^4 \phi(r_n) + \cdots , \quad \beta = \begin{cases} 1, & n > 0 \\ \frac{5}{3}, & n = 0 \end{cases}$$

$$\delta_n \phi(r_n) - \frac{\partial}{\partial r_n} \phi(r_n) = \frac{h^2}{6\nu} \frac{\partial^3}{\partial r_n^3} \phi(r_n) + \cdots , \quad \nu = \begin{cases} 1, & n > 0 \\ -\frac{1}{2}, & n = 0 \end{cases}$$

$$\mathcal{P}(r_x) - \phi(r_x) = \frac{\xi(1-\xi)}{2} h^2 \frac{\partial^2}{\partial r_x^2} \phi(r_x) + \cdots , \quad \xi = x - \mathrm{mod}\, x$$

$$^{(2)}\tilde{\psi}(t_{m+\theta}) - \psi(t_{m+\theta}) = \frac{\theta(1-\theta)}{2} (\ell_{m+1})^2 \frac{\partial^2}{\partial t_{m+\theta}^2} \psi(t_{m+\theta}) + \cdots$$

$$^{(3)}\tilde{\psi}(t_m) - \psi(t_m) = \frac{1}{3} (\ell_m^*)^2 \frac{\partial^2}{\partial t_m^2} \psi(t_m) + \cdots , \quad \ell_m^* = (\ell_m \ell_{m+1})^{1/2}$$

$$\Delta_t^{(2)} \psi(t_{m+\theta}) - \frac{\partial}{\partial t_{m+\theta}} \psi(t_{m+\theta}) = (1-2\theta) \ell_{m+1} \frac{\partial^2}{\partial t_{m+\theta}^2} \psi(t_{m+\theta}) + \frac{(1-3\theta+3\theta^2)}{6} (\ell_{m+1})^2 \frac{\partial^3}{\partial t_{m+\theta}^3} \psi(t_{m+\theta}) + \cdots$$

$$\Delta_t^{(3)} \psi(t_m) - \frac{\partial}{\partial t_m} \psi(t_m) = \frac{1}{6} (\ell_m^*)^2 \frac{\partial^3}{\partial t_m^3} \psi(t_m) + \cdots$$

and

$$\sum_{n' j m'}^{nm} P(r_n, r_{n'}, \mu_j, t_m, t_{m'} \mid \langle G \rangle) - H(r_n, t_m) = ① + ② + ③ + ④$$

where

$$① = h^2 \int_0^{r_N} 2\pi r'^2\, dr' \int_{-1}^{1} d\mu \int_0^{t_m} dt' \,\langle G(r', t')\rangle \times$$

$$\left\{\frac{F_1}{12}\nabla^4_{r_y} + \frac{F_2}{6}\frac{\partial^3}{\partial r_y^3}\right\}\langle G(r_y, t_m - t')\rangle\,,\quad r_y \in (0, r_N)$$

$$② = \frac{\pi h^5}{18} N\left(N^2 - \frac{1}{10}\right)\int_{-1}^{1} d\mu \int_0^{t_m} dt' \frac{\partial^2}{\partial \xi^2} P(r_n, \xi, \mu, t_m, t' \,|\, \langle G\rangle),\ \xi \in (0, r_N)$$

$$③ = (2/J)^2 \int_0^{\infty} \frac{\pi}{3} r'^2\, dr' \int_0^{t_m} dt' \frac{\partial^2}{\partial \eta^2} P(r_n, r', \eta, t_m, t' \,|\, \langle G\rangle),\ \eta \in (-1, 1)$$

$$④ = \ell_1^3 \left(\frac{b^{3m_2} - 1}{b^3 - 1}\right)\int_0^{\infty} \frac{\pi}{3} r'^2\, dr' \int_{-1}^{1} d\mu \frac{\partial^2}{\partial \zeta^2} P(r_n, r', \mu, t_m, \zeta \,|\, \langle G\rangle),\ \zeta \in (0, t_m).$$

Note that term ① is $O(h^2)$, ② is $O(h^2)$ for finite r_N, ③ is $O([\Delta\mu]^2)$ which may be made $O(h^2)$ by taking $J \geq 2N$. The order of ④ depends on b and m. Term ④ is $O(\ell_1^2)$ as $b \to 1$ and $O([1 + 3(b-1)^{-2}]^{-1})$ as $m \to \infty$ for finite t_m. The anticipation that $\partial^2 P/\partial t'^2$ becomes small for t' near t_{m_2} is the justification for assuming that the variable order of ④ can be effectively maintained at $O(\ell_m^2)$. With these restrictions the truncation error for **H** is $O(h^2) + O(\ell_m^2)$.

b. Thomas algorithm

Consider Equation (4) with **z** lumped into **d**; i.e., $B\mathbf{g} = \mathbf{d}$. B is tri-diagonal with diagonal elements $b_0, b_1, \ldots b_{N-1}$, subdiagonals $-a_1, -a_2, \ldots -a_{N-1}$, and supradiagonals $-c_0, -c_1, \ldots -c_{N-2}$. Normalized upper-diagonal form is obtained by calculating new coefficients

$$\left.\begin{aligned} &\alpha_0 = c_0/b_0,\ \alpha_n = c_n/e_n \\ &\beta_0 = d_0/b_0,\ \beta_n = (d_n + a_n \beta_{n-1})/e_n \end{aligned}\right\} n = 1, 2, \cdots N-1$$

where $e_n = b_n - a_n \alpha_{n-1}$. Then **g** is given directly by

$$g_N = 0,\ g_n = g_{n+1}\,\alpha_n + \beta_n \quad n = N-1,\ N-2, \cdots 1.0.$$

c. Computer programs

The computer language used for the numerical experiments is Fortran-IV. Because of storage limitations (core = 2^{15} = 32,768 words) the calculation of **G** is performed in one job segment in ALTIO mode (minimal IO buffer), and the result is written on magnetic tape; in the second job segment **G** is read from the tape in FIOCS mode and is printed, plotted, or used in subsequent calculations. To avoid long subroutine argument lists, **G**, all input parameters, and certain calculated quantities are placed in a COMMON block; those portions which are used in each subroutine are so indicated by EQUIVALENCE statements. In the first job segment **G** is stored in a 102 × 201 array.

In the first job segment the magnetic tape is first positioned with a tape manipulation subroutine. Next a subroutine for handling input reads in the necessary input parameters mentioned in the text, computes auxiliary parameters, and places them all in COMMON. This routine also has an entry provision for changing input parameters under a NAMELIST format. Then a subroutine is called which performs the computation of **G** using either Equations (2) or (3) and the methods of Section (3b). This routine calls routines for calculating G_n^0 and the term $(\mathbf{d} + \mathbf{z})$ in Equation (4).

In the second job segment the values of **G** calculated in the first segment are either printed out or plotted (with the University of Michigan plotting routine) or else made available for further computations.

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