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THE STATISTICAL THEORY OF TURBULENT FLAMES

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CONTENTS

The theory stemming from the statistical representation of turbulent flames is presented and developed, the major aim being to describe the basic processes in relatively simple flames.

Starting from conservation equations, with the assumption of low Mach number and high Reynolds number, it is shown that the properties at any point in the flame can be determined from the transport equations for the velocity U and a set of scalars ϕ: ϕ represents the species mass fractions and enthalpy. However, the solution of these equations with initial conditions and boundary conditions appropriate to turbulent flames is prohibitively difficult. Statistical theories attempt to describe the behaviour of averaged quantities in terms of averaged quantities. This requires the introduction of closure approximations, but renders a more readily soluble set of equations. A closure of

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the Reynolds-stress equations and the equation for the joint probability density function of $\boldsymbol{\phi}$ is considered. The use of the joint probability density function (p.d.f.) equation removes the difficulties that are otherwise encountered due to non-linear functions of the scalars (such as reaction rates). While the transport equation for the joint p.d.f. provides a useful description of the physics, its solution is feasible only for simple cases. As a practical alternative, a general method is presented for estimating the joint p.d.f. from its first and second moments: transport equations for these quantities are also considered therefore.

Modelled transport equations for the Reynolds stresses, the dissipation rate, scalar moments and scalar fluxes are discussed, including the effects of reaction and density variations. A physical interpretation of the joint p.d.f. equation is given and the modelling of the unknown terms is considered. A general method for estimating the joint p.d.f. is presented. It assumes that the joint p.d.f. is the statistically most likely distribution with the same first and second moments. This distribution is determined for any number of reactive or non-reactive scalars.

A. INTRODUCTION

1. *Introduction and outline*

Recently, research into turbulent flames has increased owing to a greater need for understanding and an enhanced hope of its attainment. The need stems from rising fuel costs and stricter regulation of atmospheric pollution from combustion products: the hope of gaining a better understanding of flames is mainly attributable to the qualified success of turbulence modelling, a practice that enables the velocity field and other mean properties of inert flows to be calculated. As well as causing an increase in the established literature, this research boom has resulted in several collective works (Murthy 1975; Bracco 1976; Brodkey 1975) which reflect the diversity of approaches to the subject. Workers from many fields have made their contributions and yet the ability to calculate local flame properties such as temperature is extremely limited. Many models have been proposed and many calculations performed but, with the possible exception of one special case (the idealized diffusion flame), no physically realistic and quantitatively accurate model has been demonstrated. The development of sound theories has been hindered by the paucity of relevant experimental data which has also allowed unsound theories to go without direct refutation: this in turn has led, in some quarters, to an overestimation of present abilities.

The aim of this work is to re-examine the problem of modelling turbulent flames, and to present and develop an appropriate statistical theory. In view of the unsatisfactory state of current abilities, the emphasis throughout is on determination of the basic properties of relatively simple flames. Minor species pollutant formation is not considered nor are complicating factors such as droplet fuels or soot formation.

Theoretical and experimental studies of turbulent flames have centred on idealizations of practically occurring situations. The three archetypal configurations are the jet diffusion flame corresponding to a furnace flame, the homogeneously premixed flame corresponding to a reheat system and the jet premixed flame: these are illustrated in figure 1. A tractable theory for such flames can be obtained with the assumption of a single phase, high Reynolds number, low Mach number flow. The consideration of single phase flow eliminates complications caused by fuel droplets and particles on the one hand and soot formation on the other; and, for gaseous fuels and their combustion products, the Prandtl and Schmidt numbers are not far from unity. At the high Reynolds number considered, the aerodynamics of the flow are dominated by inertial processes and, except in the immediate vicinity of solid surfaces, viscosity plays a subordinate rôle. No specific assumption is made about the reaction mechanism although, on the ground of practicality, a simple scheme is required. The assumption of low Mach number ensures that turbulent pressure fluctuations are not large enough to affect the rate of chemical reaction.

The type of theory sought is one whereby, given the physical properties of the fuel and oxidant together with appropriate boundary and initial conditions, the average velocity, temperature and species concentration fields can be determined. For laminar flows this can be accomplished by solution of the conservation equations for mass, momentum, energy and chemical species; for turbulent flows the same equations hold but, due to the widely differing length and time scales, their solution is impossible. If such a solution were obtained it would describe the detailed behaviour of the flame at every instant, including even the smallest scale of fluctuation due to turbulence. This is far more information than can be of use. The less detailed description provided by average quantities is all that is required, and it is the purpose of the theory considered to achieve this through a commensurately less complicated, soluble, set of equations. In other words, a statistical theory is sought to describe the behaviour of the flame in terms of statistical quantities.

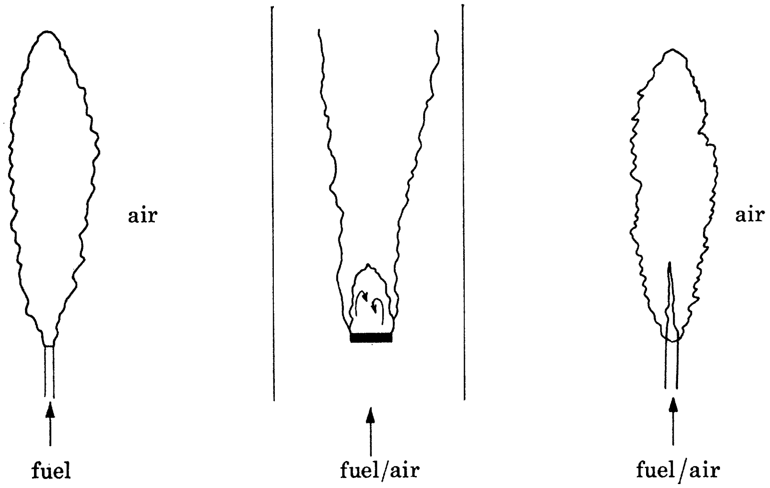

FIGURE 1. Simple turbulent flames.

In the next section, the conservation equations for mass, momentum, energy and chemical species are presented and the assumptions implemented. This results in a closed set of equations for the velocity $\boldsymbol{U}(\boldsymbol{x}, t)$ and scalar quantities $\phi(\boldsymbol{x}, t)$, species mass fractions and enthalpy. In § 3 the statistical approach is introduced with a discussion on methods of obtaining statistical averages: density-weighted ensemble averages (denoted by a tilde) are most appropriate in turbulent flames. Conservation equations for the average velocity and scalar fields, $\widetilde{\boldsymbol{U}}(\boldsymbol{x}, t)$ and $\widetilde{\phi}(\boldsymbol{x}, t)$, are not immediately soluble since they contain two types of unknown terms. First, correlations of fluctuating velocity, $\boldsymbol{u}''$, with itself or with fluctuations in the scalars ϕ'', appear in the equations, representing transport by the turbulent velocity field. Secondly, average values of density and reaction rates appear: these can be determined from the joint probability density function $p(\psi; \boldsymbol{x}, t)$.

The remainder of the paper is concerned with methods of determining these unknowns – $\widetilde{u_i'' u_j''}$, $\widetilde{u_i'' \phi_\alpha''}$ and $p(\psi; \boldsymbol{x}, t)$ – and the strategy adopted is discussed in § 4. Part B, §§ 5–9, is concerned with 'turbulence models' which can be used to determine the Reynolds stresses, $\widetilde{u_i'' u_j''}$, the scalar fluxes,

$\widetilde{u_i''\phi_\alpha''}$, and scalar variances, $\widetilde{\phi_\alpha''\phi_\beta''}$. The transport equations for these quantities are, and will remain, central to calculation methods for turbulent flames.

In a laminar flame, a complete description of the chemical composition of the gases at any point is provided by a knowledge of the mass fractions $\boldsymbol{\phi}(\boldsymbol{x}, t)$, say, of every species. Reaction and mixing cause the composition to vary from point to point. For a turbulent flame, a complete statistical description of the chemical composition is provided by the joint probability density function $p(\boldsymbol{\psi}; \boldsymbol{x}, t)$ where

$$p(\boldsymbol{\psi}; \boldsymbol{x}, t)\, \mathrm{d}\boldsymbol{\psi}$$

represents the probability of $\boldsymbol{\phi}(\boldsymbol{x}, t)$ being in the range

$$\boldsymbol{\psi} < \boldsymbol{\phi}(\boldsymbol{x}, t) < \boldsymbol{\psi} + \mathrm{d}\boldsymbol{\psi}.$$

$\boldsymbol{\psi}$ is the set of independent variables corresponding to the dependent scalar variables, $\boldsymbol{\phi}(\boldsymbol{x}, t)$: a given value of $\boldsymbol{\psi}$ corresponds to a gas mixture of a given composition, and hence $\boldsymbol{\psi}$-space is termed the composition space. $p(\boldsymbol{\psi}; \boldsymbol{x}, t)$ represents the statistical distribution of compositions, and phenomena that affect chemical composition (reaction and mixing) can be regarded as affecting this distribution in composition space.

In part C, §§ 10–12, the properties and behaviour of the joint probability density function are studied. A consideration of the transport equation for $p(\boldsymbol{\psi}; \boldsymbol{x}, t)$ throws light on his behaviour but, in all but the simplest of cases, the equation appears prohibitively difficult to solve. Consequently, an alternative method of determining $p(\boldsymbol{\psi}; \boldsymbol{x}, t)$ is required. The method proposed is, simply, to assume that $p(\boldsymbol{\psi}; \boldsymbol{x}, t)$ is the statistically most likely distribution. In § 12 this distribution is determined as a function of the reaction rates and of the first and second moments, $\tilde{\phi}_\alpha$ and $\widetilde{\phi_\alpha''\phi_\beta''}$. Thus, rather than solving the transport equation for $p(\boldsymbol{\psi}; \boldsymbol{x}, t)$, its most likely value can be deduced from the solution of the far simpler transport equations for $\tilde{\phi}_\alpha$ and $\widetilde{\phi_\alpha''\phi_\beta''}$.

2. *Formulation*

The chemical and thermodynamic properties of a reacting system can be characterised by the mass fraction of each chemical species, m_α, the enthalpy, h, and the pressure p; an equation of state relates these quantities to the density. The velocity, U, completes the description of the system. These quantities obey the following conservation equations:

conservation of mass
$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_i}{\partial x_i} = 0, \tag{2.1}$$

conservation of momentum
$$\frac{\partial \rho U_j}{\partial t} + \frac{\partial \rho U_i U_j}{\partial x_i} = -\frac{\partial \tau_{ij}}{\partial x_i} - \frac{\partial p}{\partial x_j} + \rho g_j, \tag{2.2}$$

conservation of chemical species
$$\frac{\partial \rho m_\alpha}{\partial t} + \frac{\partial \rho U_i m_\alpha}{\partial x_i} = -\frac{\partial J_i^\alpha}{\partial x_i} + \rho S_\alpha, \tag{2.3}$$

conservation of enthalpy
$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho U_i h}{\partial x_i} = -\frac{\partial J_i^h}{\partial x_i} + \rho S_h, \tag{2.4}$$

where g_j is the component of gravitational acceleration in the j-direction, τ_{ij}, J_i^α and J_i^h are the mass fluxes of the quantities involved owing to molecular transport, and S_α and S_h are the mass rates of addition per unit volume. These quantities are (in principle) known functions of the physical and chemical properties of the gases involved and the formulation is completed by the equation of state,

$$\rho = \rho(\boldsymbol{m}, h, p), \tag{2.5}$$

where $\boldsymbol{m}$ denotes the set of species mass fractions. Other quantities, such as temperature T, can be determined from similar, auxiliary, relations,

$$T = T(\boldsymbol{m}, h, p). \tag{2.6}$$

S_α is the mass rate of addition of species α due to chemical reaction. The reaction rates, and hence S_α, are algebraic functions of p, ρ, T and $\boldsymbol{m}$. ρ and T are given in terms of p, h and $\boldsymbol{m}$ by equations (2.5) and (2.6), and so S_α can be expressed as a function of p, $\boldsymbol{m}$ and h. The assumption of low Mach number, Ma, is invoked in order to remove the dependence of S_α on pressure variations, Δp, caused either by the mean flow or by turbulent fluctuations. The magnitude of such variations can be estimated as follows:

$$\Delta p \propto \rho U^2 = Ma^2(\rho a^2), \tag{2.7}$$

where U is a characteristic velocity and a is the speed of sound. In terms of the ratio of specific heats ($\gamma \approx 1.4$, say) the speed of sound is

$$a = (\gamma p/\rho)^{\frac{1}{2}}, \tag{2.8}$$

which leads to

$$\Delta p/p \propto Ma^2. \tag{2.9}$$

Thus, while S_α depends upon the absolute level of pressure, its dependence on pressure fluctuations can be ignored at low Mach number.

Enthalpy, h, represents the thermodynamic and chemical (but not mechanical) energy per unit volume, and its source S_h can be caused by two agencies – radiation and the conversion of mechanical energy to heat by compressibility and viscous dissipation. The treatment of radiant heat transfer in flames is a difficult task and outside the scope of the present work. It is assumed, therefore, that the contribution of radiation to S_h either is known in terms of p, $\boldsymbol{m}$ and h or is negligible. (For small flames, such as those in laboratories, heat loss by radiation is usually a negligible fraction of the total heat flow.)

The assumption of low Mach number allows the neglect of the transfer of mechanical energy to heat. The mechanical energy (per unit mass), $\frac{1}{2}U^2$, is small compared with the heat content, $C_p T$:

$$\tfrac{1}{2}U^2/C_p T \approx Ma^2\tfrac{1}{2}(\gamma - 1). \tag{2.10}$$

The left hand side of equation (2.10) represents the fractional rise in temperature, $\Delta T/T$, that would result from all the mechanical energy being converted into heat. Clearly, at low Mach number this is negligible compared with the temperature rise due to combustion.

In inert, isothermal flows of ideal gases, the viscous stress tensor is given by Newton's law of viscosity,

$$\tau_{ij} = -\mu(\partial U_i/\partial x_j + \partial U_j/\partial x_i); \tag{2.11}$$

and, for binary mixtures, the species mass flux J_i^α is given by Fick's law,

$$J_i^\alpha = -\Gamma \partial m_\alpha/\partial x_i. \tag{2.12}$$

In flames, with many chemical species and steep gradients of density and temperature, these processes are far more complicated; quantities diffuse down gradients other than their own and the diffusion coefficients can be strong (though not simple) functions of the thermodynamic variables. It is possible to write a general expression for these processes but the complexity this would cause in the ensuing manipulations, if not making the equations intractable, would certainly result in attention being paid to the processes out of all proportion to their physical importance. Further, at the end of such analysis, drastic simplifications would be required in order to make the resultant equations practically solvable. In fact, the models presented below make no reference to laminar viscosities and diffusivities at all. It is only sensible, therefore, to make simplifying assumptions at this stage rather than after a great deal of algebraic manipulation. Consequently, simple gradient diffusion given by equations (2.11) and (2.12) will be employed.

Some justification for this expedient assumption is provided by the following three points.

(i) The assumption is not that the molecular processes are described by simple gradient diffusion for this is unlikely to be true. Rather, it is assumed that the behaviour of the equations on all but the smallest scales is independent of the detailed form of the diffusion. This, clearly, is a far weaker assumption.

(ii) Even if the details of the molecular processes have some influence, they are unlikely to be rate-controlling. Molecular action is only significant on small length-scales and the process of scale-reduction – whereby the length scales of the turbulent fluctuations are decreased – is an inertial process and therefore independent of viscosity and diffusivity.

(iii) In pragmatic vein, until a convincing theory is obtained based upon the simplified equations there is little merit in considering a more complicated set.

The assumptions made allow equations (2.2)–(2.5) to be rewritten as:

$$\frac{\partial \rho U_j}{\partial t}+\frac{\partial \rho U_i U_j}{\partial x_i}=\frac{\partial}{\partial x_i}\mu\left(\frac{\partial U_i}{\partial x_j}+\frac{\partial U_j}{\partial x_i}\right)-\frac{\partial p}{\partial x_j}+\rho g_j, \tag{2.13}$$

$$\frac{\partial \rho \phi_\alpha}{\partial t}+\frac{\partial \rho U_i \phi_\alpha}{\partial x_i}=\frac{\partial}{\partial x_i}\Gamma\frac{\partial \phi_\alpha}{\partial x_i}+\rho S_\alpha, \tag{2.14}$$

and

$$\rho=\rho(\boldsymbol{\phi}), \tag{2.15}$$

where ϕ_α represents one of the scalars (m_α or h) and ρ and S_α are known functions.

3. *Statistical equations*

Equations (2.1) and (2.13)–(2.15) form a closed set. With initial conditions, $\boldsymbol{U}(\boldsymbol{x}, t_0)$ and $\boldsymbol{\phi}(\boldsymbol{x}, t_0)$, and boundary conditions, $\boldsymbol{U}(\boldsymbol{x}_\mathrm{b}, t)$ and $\boldsymbol{\phi}(\boldsymbol{x}_\mathrm{b}, t)$, then $\boldsymbol{U}$ and $\boldsymbol{\phi}$ are determined within the boundary by these equations for times greater than t_0. Analytic solutions have only been obtained for simple laminar flows. In general, numerical solution seems to be the only way but, for turbulent flows, even this is restricted to very low Reynolds number, Re, because of computer limitations. And the computer time required to solve the equations increases (at least) as $\mathrm{Re}^{\frac{11}{4}}$. This indicates that the direct approach is ill conceived since the mean quantities of interest are found to be, at most, weak functions of Reynolds number. Since it is average quantities that are of interest, an immediately apparent alternative approach is to consider the averaged conservation equations.

There is some difficulty in providing a definition of average quantities that is easy to measure and has the desired mathematical properties. Here ensemble (or realization) averaging, indicated by angular brackets, is used:

$$\langle \phi(\boldsymbol{x}, t)\rangle \equiv \lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N}\phi^{(n)}(\boldsymbol{x}, t), \tag{3.1}$$

where $\phi^{(n)}(\boldsymbol{x}, t)$ is the value of ϕ at $\boldsymbol{x}$ and t in the nth of N similar realizations. Nearly all the relevant experiments are performed in statistically stationary flows (that is, $\partial\langle\phi(\boldsymbol{x}, t)\rangle/\partial t = 0$) in which case the more easily measured time averages are equal to ensemble averages.

From the definition of ensemble averaging, it follows that

$$\langle\langle\phi\rangle\rangle = \langle\phi\rangle, \tag{3.2}$$

$$\left\langle\frac{\partial\phi}{\partial t}\right\rangle = \frac{\partial\langle\phi\rangle}{\partial t}, \quad \left\langle\frac{\partial\phi}{\partial x_i}\right\rangle = \frac{\partial\langle\phi\rangle}{\partial x_i}, \tag{3.3}$$

and

$$\langle\phi+\theta\rangle = \langle\phi\rangle+\langle\theta\rangle. \tag{3.4}$$

With the further definition of fluctuating values,

$$\phi'(\boldsymbol{x}, t) \equiv \phi(\boldsymbol{x}, t) - \langle\phi(\boldsymbol{x}, t)\rangle, \tag{3.5}$$

it follows that

$$\langle\phi'\rangle = 0, \tag{3.6}$$

$$\langle\phi'\theta'\rangle = \langle\phi\theta'\rangle = \langle\phi\theta\rangle - \langle\phi\rangle\langle\theta\rangle, \tag{3.7}$$

and similar relations for multiples of three and more quantities.

Decomposing each variable into its mean and fluctuating component, substituting into equation (2.13) and ensemble averaging yields an equation for the conservation of mean momentum:

$$\begin{aligned}\frac{\partial}{\partial t}(\langle\rho\rangle\langle U_j\rangle+\langle\rho u_j\rangle)+\frac{\partial}{\partial x_i}(\langle\rho\rangle\langle U_i\rangle\langle U_j\rangle+\langle\rho\rangle\langle u_i u_j\rangle+\langle U_i\rangle\langle\rho u_j\rangle+\langle U_j\rangle\langle\rho u_i\rangle+\langle\rho' u_i u_j\rangle)\\ =\frac{\partial}{\partial x_i}\mu\left(\frac{\partial}{\partial x_j}\langle U_i\rangle+\frac{\partial}{\partial x_i}\langle U_j\rangle\right)-\frac{\partial\langle p\rangle}{\partial x_j}+\langle\rho\rangle g_j.\end{aligned} \tag{3.8}$$

($\boldsymbol{u}$ rather than $\boldsymbol{U}'$ is used for fluctuating velocity.) It is immediately apparent that, in the process of decomposing and averaging, extra terms are generated and the equation loses its straightforward physical interpretation. In hindsight, part of the reason for this is readily seen. In the momentum equation (2.13), which can be regarded as an equation for U_j, ρU_j represents the momentum per unit volume. The mean momentum per unit volume is $\langle\rho\rangle\langle U_j\rangle+\langle\rho u_j\rangle$ and so the subject of equation (3.8) can be thought of as $\langle U_j\rangle+\langle\rho u_j\rangle/\langle\rho\rangle$: the equation is commensurately complicated.

Simpler and more easily interpreted equations are obtained by decomposing quantities into a mean $\tilde{\phi}$, and fluctuating component, ϕ'', such that $\langle\rho\rangle\tilde{m}_\alpha$ is the mean mass of species α per unit volume and so on. This is achieved through density-weighted averaging or Favre averaging (Favre 1969) which defines $\tilde{\phi}$ and ϕ'' by

$$\langle\rho\rangle\tilde{\phi} \equiv \langle\rho\phi\rangle, \tag{3.9}$$

and

$$\phi'' \equiv \phi - \tilde{\phi}. \tag{3.10}$$

Equation (3.9), as well as defining $\tilde{\phi}$, defines the process of density-weighted averaging: thus, for example,

$$\langle\rho\rangle\widetilde{\phi''} = \langle\rho\phi''\rangle = 0, \tag{3.11}$$

and

$$\langle\rho\rangle\widetilde{\phi''\psi''} = \langle\rho\phi''\psi''\rangle. \tag{3.12}$$

Note, however, that in general $\langle\phi''\rangle$ is non-zero.

By using density-weighted averaging, the conservation equation for mean momentum becomes,

$$\frac{\partial}{\partial t}\langle\rho\rangle\,\tilde{U}_j+\frac{\partial}{\partial x_i}(\langle\rho\rangle\,\tilde{U}_i\,\tilde{U}_j+\langle\rho u_i'' u_j''\rangle)=\frac{\partial}{\partial x_i}\mu\left(\frac{\partial\langle U_i\rangle}{\partial x_j}+\frac{\partial\langle U_j\rangle}{\partial x_i}\right)-\frac{\partial\langle p\rangle}{\partial x_j}+\langle\rho\rangle\,g_j. \tag{3.13}$$

In this equation, the first term represents the change with time of the mean j-direction momentum per unit volume; $\partial(\langle\rho\rangle\,\tilde{U}_i\,\tilde{U}_j)/\partial x_i$ represents the net loss due to mean flow convection while $\partial\langle\rho u_i'' u_j''\rangle/\partial x_i$ is the net loss due to turbulent convection. The first term on the right hand side represents a gain due to molecular diffusion and is negligible at high Reynolds number: $\langle U_j\rangle$ is, at most, a weak function of Reynolds number whereas μ is inversely proportional. The final terms represent the mean force in the j-direction per unit volume.

Equations (2.1) and (2.13)–(2.15) provide a closed set of equations. Their mean counterparts (omitting the negligible molecular diffusion terms) are:

$$\frac{\partial\langle\rho\rangle}{\partial t}+\frac{\partial\langle\rho\rangle\,\tilde{U}_i}{\partial x_i}=0, \tag{3.14}$$

$$\frac{\partial}{\partial t}\langle\rho\rangle\,\tilde{U}_j+\frac{\partial}{\partial x_i}(\langle\rho\rangle\,\tilde{U}_i\,\tilde{U}_j+\langle\rho u_i'' u_j''\rangle)=-\frac{\partial\langle p\rangle}{\partial x_j}+\langle\rho\rangle\,g_j, \tag{3.15}$$

$$\frac{\partial}{\partial t}\langle\rho\rangle\tilde{\phi}_\alpha+\frac{\partial}{\partial x_i}(\langle\rho\rangle\,\tilde{U}_i\tilde{\phi}_\alpha+\langle\rho u_i''\phi_\alpha''\rangle)=\langle\rho\rangle\,\tilde{S}_\alpha(\phi), \tag{3.16}$$

and

$$\langle\rho\rangle=\langle\rho(\phi)\rangle. \tag{3.17}$$

(The derivation of all equations quoted can be found in the appendix.) It may be noted that $\langle\rho\rangle\,\widetilde{u_i''u_j''}$ could be written for $\langle\rho u_i'' u_j''\rangle$ and similarly for $\langle\rho u_i''\phi_\alpha''\rangle$.

The quantities appearing in these equations may be considered in three groups:

(i) $\tilde{U}, \langle p\rangle, \quad \tilde{\phi}$,

(ii) $\langle\rho u_i'' u_j''\rangle, \quad \langle\rho u_i''\phi_\alpha''\rangle$,

and (iii) $\langle\rho(\phi)\rangle, \quad \tilde{S}_\alpha(\phi)$.

Group (i) comprises the mean quantities which it is the objective to determine. Equations (3.14)–(3.16) can be considered equations for $\tilde{U}$ and $\tilde{\phi}$, $\langle p\rangle$ being a function of $\tilde{U}$, and then groups (ii) to (iii) quantities are 'unknowns'. The quantities in group (ii) are density-weighted velocity–velocity or velocity–scalar correlations which are zero for a laminar flow but non-zero for turbulent flows whether reactive or not. The principle aim of turbulence modelling is to provide a means of determining these.

The quantities in the third group are functions of the scalars alone and their determination if trivial in laminar flows. $\rho(\phi)$ and $S_\alpha(\phi)$ are known functions and, typically, S is highly nonlinear. Consequently,

$$\tilde{S}_\alpha(\phi)\neq S_\alpha(\tilde{\phi}); \tag{3.18}$$

indeed, the two sides of this inequality can differ by several orders of magnitude. The mean reaction rates (and any other function) can be evaluated from the joint probability density function (p.d.f.) of the scalars by

$$\langle\rho\rangle\,\tilde{S}_\alpha(\phi)=\int p(\psi)\,\rho(\psi)\,S_\alpha(\psi)\,\mathrm{d}\psi. \tag{3.19}$$

(It may be recalled that ψ represents the composition space and $p(\psi)\,\mathrm{d}\psi$ is the probability that ϕ lies in the range $\psi<\phi<\psi+\mathrm{d}\psi$.) Here, the determination of $p(\psi)$ is regarded as the principal aim of combustion modelling. Of course, $p(\psi)$ contains far much more information than is required – that is, $\tilde{S}_\alpha(\phi)$ and $\langle\rho(\phi)\rangle$ – and so it could be claimed that the determination of $p(\psi)$ is commensurately more difficult than the determination of $\tilde{S}_\alpha(\phi)$ and $\langle\rho(\phi)\rangle$. In fact, because $p(\psi)$ contains all the statistical information about the scalars at a point, its determination is in many ways more simple.

At this stage the general problem and objective can be stated more clearly. Equations (2.1) and (2.13)–(2.15) describe the detailed behaviour of turbulent flames but, because they contain so much detail, they cannot be solved directly. However, a statistical description in terms of average quantities, $\langle U\rangle$ and $\langle\phi\rangle$, is adequate for nearly all purposes. (In fact, for variable density flows, it is more convenient and physically more meaningful to consider the density-weighted mean quantities, $\tilde{U}$ and $\tilde{\phi}$.) Equations (3.14)–(3.16) can be solved for $\tilde{U}$ and $\tilde{\phi}$ if the turbulent fluxes ($\langle\rho u_i'' u_j''\rangle$ and $\langle\rho u_i'' \phi_\alpha''\rangle$) and the mean reaction rates and density are known: a knowledge of the joint probability distribution of the scalars, $p(\psi)$, is sufficient to determine these latter two quantities. Thus, the description of turbulent flames sought can be achieved with a knowledge of the turbulent fluxes and the joint p.d.f. of the scalars.

4. *Closure strategy*

In the transport equations for a group of statistical quantities, quantities appear that are not contained within the group. This is the closure problem which exists for all groups, and combinations of groups, of statistical quantities. It reflects the fact that statistical quantities can provide only a partial description of turbulence and that they are affected by influences other than those that they describe. Statistical theories effect closure by approximating these influences in terms of the statistical quantities within the group considered, thus equalizing the numbers of quantities and equations.

Statistical theories are different in nature to deterministic theories. From the instantaneous conservation equations, the future state of a flow can (in principle) be determined precisely, given a precise knowledge of the initial and boundary conditions. Given only statistical information about the initial and boundary conditions, the flow is not completely specified and so the future state, even of statistical quantities, is not completely determined. In other words, there is an uncertainty in the future values of statistical quantities due to the influence of the remaining, unknown, initial and boundary conditions. The most that can be expected of a statistical theory, therefore, is to provide an estimate of the future values within this uncertainty. An accurate theory is only possible if this uncertainty is small which, in turn, requires that the influence of the unknown initial and boundary conditions be small. Consequently, a high-level closure (which considers many statistical quantities) is potentially more accurate than a low level closure since it affords a more complete flow specification. A closure developed for only one class of flow is also potentially more accurate, since then the unspecified boundary conditions are, to an extent, implied by those specified. The present restriction to flows remote from walls is advantageous in this respect.

A high-level closure is 'potentially' more accurate, but this potential must be realised. If a given level of closure is adequate in a given flow, then the unknowns can be accurately represented as functions of the known quantities. The task of the theory is to determine the precise form of such functions. The following factors bear upon this task:

(*a*) physical insight,

(*b*) available experimental data

and

(*c*) ease of solution of the resultant equations.

Both available data and the ease of solution of the equations decreases with increasing levels of closure. Consequently, the full potential of high-level closures is unlikely to be realized since testing is difficult. Physical insight tends to increase to a maximum at some level of closure and then decrease rapidly: the concepts associated with a low-level closure may be too crude to provide a physically-based understanding of the phenomena, while at a high level, the complex statistical quantities involved and the lack of data result in a poor picture of the physics.

The optimum level at which to close the statistical equations of § 3 is now considered. In fact, more than one level is usually appropriate: concepts appropriate to one level can be used to effect closure at another while, for practical flow calculations, a lower level (with more easily solved equations) may be preferable.

There is little doubt that, for constant-density flows, a second order closure represents the optimum level. In this, transport equations are solved for all second moments (that is, the group (ii) quantities $\langle \rho u''_i u''_j \rangle$, $\langle \rho u''_i \phi''_\alpha \rangle$ and $\langle \rho \phi''_\alpha \phi''_\beta \rangle$) and for ϵ, the dissipation rate of turbulent kinetic energy. That this is the optimum level is a consensus view. Data of $\widetilde{u''_i u''_j}$ are available for many flows while the smaller amount of data of $\widetilde{u''_i \phi''_\alpha}$ and $\widetilde{\phi''_\alpha \phi''_\beta}$ is almost adequate for modelling purposes: more physical insight is provided than from a consideration of $\tilde{U}$ and $\tilde{\phi}$ alone, and the resultant equations are not too difficult to solve, at least for the simple flows for which there are data.

The closure of the Reynolds-stress, dissipation and scalar equations is considered in §§ 5, 6 and 7 and the effects of variable density in § 8. The mean quantities, all second moments and the dissipation, ϵ, are regarded as 'known'. Closure approximations for the unknowns in terms of the knowns renders a closed set of equations. Specific closure approximations for all the unknowns are discussed.

The potential accuracy of this set of equations depends on the extent to which the unknowns are uniquely determined by the knowns; or, from a different point of view, the equations are likely to become inaccurate for flow regions where this determinism does not exist. The accuracy of the models is assessed in § 9. No model has yet realized the full potential of Reynolds-stress closures and consequently it is not possible to establish unequivocally whether this level of closure is sufficient to describe a given flow accurately. That is, when discrepancies are found between experiment and theory, it is not always possible to distinguish between inaccurate modelling and the insufficiency of the level of closure. If it is the former, then a refined model will calculate the flow accurately, if it is the latter, then there can be no remedy within that level of closure. It is suggested that second order closures are sufficient for simple flows (jets, for example) and that for more complex flows the case is, as yet, unproved.

It has already been shown that the joint p.d.f. $p(\psi)$ provides a complete description of the reacting scalar field and that a knowledge of $\widetilde{u''_i u''_j}$ and $p(\psi)$ is sufficient to effect a closure. The transport equation for $p(\psi)$ has the advantage over equations for moments of ϕ that chemical reaction is expressed in closed form. Other terms have to be modelled and this is discussed in § 11. The modelled equation for $p(\psi)$ can be solved in simple cases and an ever increasing body of experimental data is available. However, the difficulty in solving the equation escalates rapidly as the complexity of the flow and the number of scalars increases. Consequently, a simpler set of equations is required in the general case.

A simpler set of equations inevitably contains less information, and the deficit must be made up by assumptions, either explicit or implicit. In § 12, a general method of determining $p(\psi)$ from given information is presented: the explicit assumption is, simply, that $p(\psi)$ is the statistically most likely distribution, subject to available information. The minimum amount of information required is mean values, $\tilde{\phi}$, all second moments, $\widetilde{\phi''_\alpha \phi''_\beta}$, and the reaction rates, $S_\alpha(\psi)$. From this, a p.d.f. is deduced which has the correct first and second moments and accounts for the effects of reaction on the distribution. Thus, rather than solving the transport equation for $p(\psi)$, equations for $\tilde{\phi}$ and $\widetilde{\phi''_\alpha \phi''_\beta}$ are solved and $p(\psi)$ is deduced from the resulting values. As a lower order closure, and a degenerate form of the transport equation for $p(\psi)$, this method is ideal since any amount of information (e.g. third and fourth moments) can be included. Whether more than second moments are required is a question to be answered by future experience.

B. TURBULENCE MODELS

5. *The Reynolds-stress equation*

In this and the next three sections turbulence models for determining the Reynolds stresses and scalar second moments in constant-density flows are considered. The restriction to constant density greatly simplifies the algebra and allows a larger body of established knowledge, both experimental and theoretical, to be admitted. This having been done, the necessary extension to variable-density flows is discussed in § 8. The practice of density-weighted averaging allows most of the modelling to be transferred directly and then the major effects of density fluctuations are accounted for implicitly. Additional effects can be identified and are discussed. The model equations are assessed in § 9 in an attempt to determine the types of flow for which this level of closure is adequate. The accuracy of some of the model equations can be assessed from comparison with experimental data but much of the modelling, especially that pertaining to scalars in variable-density flow, has yet to be tested.

In constant-density flows, the Reynolds-stress equation is

$$\begin{aligned}\rho\frac{\partial}{\partial t}\langle u_j u_k\rangle &+ \rho\langle U_i\rangle\frac{\partial}{\partial x_i}\langle u_j u_k\rangle + \rho\frac{\partial}{\partial x_i}\langle u_i u_j u_k\rangle \\ &= -\left\langle u_j\frac{\partial p'}{\partial x_k}\right\rangle - \left\langle u_k\frac{\partial p'}{\partial x_j}\right\rangle + \mu\left\langle u_j\frac{\partial^2 u_k}{\partial x_i^2}\right\rangle + \mu\left\langle u_k\frac{\partial^2 u_j}{\partial x_i^2}\right\rangle \\ &\quad -\rho\langle u_j u_i\rangle\frac{\partial}{\partial x_i}\langle U_k\rangle - \rho\langle u_k u_i\rangle\frac{\partial}{\partial x_i}\langle U_j\rangle. \qquad (5.1)\end{aligned}$$

Three types of unknowns appear: the gradient of the triple correlation represents turbulent convection of the Reynolds stresses, there are two pressure–interaction terms and two involving molecular diffusion. The final terms, which are known, account for the production of the Reynolds stress by the mean velocity gradients.

The terms involving molecular diffusion can be dealt with summarily: they can be re-expressed as

$$\mu\left\langle u_j\frac{\partial^2 u_k}{\partial x_i^2}\right\rangle + \mu\left\langle u_k\frac{\partial^2 u_j}{\partial x_i^2}\right\rangle = \mu\frac{\partial^2\langle u_j u_k\rangle}{\partial x_i^2} - \rho\epsilon_{jk}. \qquad (5.2)$$

The first term on the right hand side of (5.2) represents transport due to molecular diffusion and is negligible at the high Reynolds number considered. The second term,

$$\epsilon_{jk} = 2\frac{\mu}{\rho}\left\langle\frac{\partial u_j}{\partial x_i}\frac{\partial u_k}{\partial x_i}\right\rangle, \tag{5.3}$$

again at high Reynolds number has negligible off-diagonal components (Lumley 1975*a*) and can therefore be written,

$$\epsilon_{jk} = \tfrac{2}{3}\epsilon\delta_{jk}, \tag{5.4}$$

where

$$\epsilon \equiv \left\langle\frac{\mu}{\rho}\left(\frac{\partial u_i}{\partial x_j}\right)^2\right\rangle = \tfrac{1}{2}\epsilon_{ii}. \tag{5.5}$$

ϵ is the rate of dissipation of turbulent kinetic energy ($k \equiv \frac{1}{2}\langle u_i u_i\rangle$) and, as may be seen from equation (5.5), it is non-negative. Thus, the effect of molecular action is to extract energy equally from the three normal stresses without affecting the shear stresses.

In the type of closure considered, ϵ is calculated from its own transport equation which is treated separately in the next section.

Attention is now turned to the pressure–interaction terms which can be decomposed as follows:

$$-\left\langle u_j\frac{\partial p'}{\partial x_k}\right\rangle - \left\langle u_k\frac{\partial p'}{\partial x_j}\right\rangle = \left\langle p'\left(\frac{\partial u_j}{\partial x_k}+\frac{\partial u_k}{\partial x_j}\right)\right\rangle - \frac{\partial}{\partial x_i}\left(\langle u_k p'\rangle\delta_{ij} + \langle u_j p'\rangle\delta_{ik}\right). \tag{5.6}$$

The first term is the pressure–rate of strain correlation which contracts to zero, since $\partial u_j/\partial x_j$ is zero. (The variable-density case, in which this is not so, is considered in § 8.) That the term contracts to zero indicates that it has no effect upon the trace of the Reynolds-stress tensor (that is, (twice) the kinetic energy): it serves to redistribute energy from one component to another. The second term in equation (5.6) represents transport and is zero, therefore, in homogeneous turbulence.

Lumley (1975*b*) has pointed out that the decomposition of the pressure-interaction terms into a deviatoric part (zero trace) and a transport part is not unique. This means that the pressure–rate of strain term may also contribute to transport and, conversely, the transport term in (5.6) may serve to redistribute energy among the Reynolds stresses. For homogeneous turbulence there is no ambiguity since all transport terms are zero.

Chou (1945) has shown that the fluctuating pressure p' has contributions from the turbulence alone, p'_1, and from the combination of turbulence and mean velocity gradients, p'_2. Consequently, models of the pressure–rate of strain term generally contain two contributions: one due to p'_1 and the other due to p'_2. Launder, Reece & Rodi (1975) follow Rotta (1951) in modelling the first part as

$$\left\langle p'_1\left(\frac{\partial u_j}{\partial x_k}+\frac{\partial u_k}{\partial x_j}\right)\right\rangle = -C_1\rho\epsilon a_{jk}, \tag{5.7}$$

where a_{ij} is the normalized anisotropy tensor,

$$a_{ij} = \langle u_i u_j\rangle/k - \tfrac{2}{3}\delta_{ij}, \tag{5.8}$$

and C_1 is taken to be a constant ($C_1 = 1.5$).

A more detailed study of the term has been undertaken by Lumley & Newman (1977) who propose a complex expression which cannot be written explicitly. It does, however, predict the correct behaviour in all the homogeneous shear-free flows for which data are available. The major implication of Lumley & Newman's work for the simpler model (5.7) is that C_1 cannot be a constant. An invariant measure of the anisotropy is $\Pi \equiv a_{ij}\,a_{ji}$: as Π tends to zero, the turbulence becomes isotropic and, it is shown, C_1 tends to unity. On the other hand Π has a maximum possible value corresponding to two dimensional turbulence which, in principle, is stable which again gives $C_1 = 1$. Thus, if C_1 is to differ from unity, it must be a nonlinear function of Π.

Models for the second part of the redistribution term have been proposed by several workers, notably Lumley & Khajeh-Nouri (1974), Launder, Reece & Rodi (1975) and Lin & Wolfshtein (1977). On the assumption that the term is a linear combination of velocity gradients and Reynolds stresses, Launder, Reece & Rodi deduced the following form:

$$\left\langle p_2'\left(\frac{\partial u_j}{\partial u_k}+\frac{\partial u_k}{\partial x_j}\right)\right\rangle = -\tfrac{1}{11}(C_2+8)\,(P_{jk}-\tfrac{2}{3}P\delta_{jk}) \\ -\tfrac{1}{55}(30C_2-2)\,\rho k\left(\frac{\partial}{\partial x_k}\langle U_j\rangle+\frac{\partial}{\partial x_j}\langle U_k\rangle\right)-\tfrac{1}{11}(8C_2-2)\,(D_{jk}-\tfrac{2}{3}P\delta_{jk}), \quad (5.9)$$

where P_{jk} is the production of $\langle u_j\,u_k\rangle$,

$$P_{jk} \equiv -\rho\langle u_j\,u_i\rangle\,\partial\langle U_k\rangle/\partial x_i-\rho\langle u_k\,u_i\rangle\,\partial\langle U_j\rangle/\partial x_i, \quad (5.10)$$

$$D_{jk} \equiv -\rho\langle u_j\,u_i\rangle\,\partial\langle U_i\rangle/\partial x_k-\rho\langle u_k\,u_i\rangle\,\partial\langle U_i\rangle/\partial x_j, \quad (5.11)$$

and P, the production of kinetic energy, is given by

$$P = \tfrac{1}{2}P_{ii}. \quad (5.12)$$

The assumption of linearity allows (5.9) to be written with only one undetermined quantity, C_2, which is held to be a constant ($C_2 = 0.4$). Since there are no measurements of the term, nor are there likely to be, there would be large uncertainties in prescribing functions or constants in a more complicated model. Also, for the same reason, the accuracy of (5.9) cannot be determined directly but can only be surmised from the behaviour of a complete model. Consequently, such an appraisal is deferred to § 9.

Turbulent transport of the Reynolds stresses is caused by gradients in the triple correlations $\langle u_i\,u_j\,u_k\rangle$ and in the pressure–velocity correlations $\langle u_i p'\rangle$. As mentioned above, gradients in $\langle u_i p'\rangle$ may also cause redistribution. Most workers have assumed that the contribution of $\langle u_i p'\rangle$ to transport is negligible. This is an expedient assumption since there are no data of $\langle u_i p'\rangle$ by which a model can be tested. There are data of the triple correlation with which Cormack, Leal & Seinfeld (1978) compared the performance of four models; that of Shir (1973):

$$\langle u_i\,u_j\,u_k\rangle = -\,(C_{s1}\,k^2/\epsilon)\,\partial\langle u_i\,u_j\rangle/\partial x_k, \quad (5.13)$$

that of Daly & Harlow (1970)†:

$$\langle u_i\,u_j\,u_k\rangle = -\,(C_{s2}\,k/\epsilon)\,\langle u_k\,u_l\rangle\,(\partial\langle u_i\,u_j\rangle/\partial x_l) \quad (5.14)$$

and the more complicated proposals of Hanjalić & Launder (1972) and of Lumley & Khajeh-Nouri (1974). Cormack *et al.* concluded that the Lumley & Khajeh-Nouri model produced the best agreement but that it is too complicated for practical use. The Hanjalić & Launder model, being second best, was recommended for use. Also the optimum values of the constants in equations (5.13) and (5.14) were found to be $C_{s1} = 0.0368$ and $C_{s2} = 0.13$.

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† As written, equations (5.13) and (5.14) are improper in that the left hand sides are symmetric in all indices while the right hand sides are not: however, differentiation with respect to x_k yields the contribution of the triple correlation to the transport, and then both sides are symmetric in i and j. Also, it should be noted that equation (5.13) is not exactly the model proposed by Shir.

Launder, Reece & Rodi (1975) compared the performance of the Daly & Harlow and the Hanjalić & Launder models in a variety of shear flows. The Daly & Harlow model produced better results in general and, because of its relative simplicity, was preferred. However, the constant used was $C_{s2} = 0.21$ and, more recently, Launder & Morse (1977) give $C_{s2} = 0.22$. There is a similar discrepancy in the value attributed to the constant in Shir's model: the best-fit value given by Cormack *et al.* is $C_{s1} = 0.0368$ and yet for consistency with the constants in lower-order closures (e.g. Jones & Launder 1972) the value should be $C_{s1} = 0.09$. The lower values of C_{s1} and C_{s2} come from direct comparison with the triple correlations while the higher values produce the correct amount of transport in shear flows. Although the evidence is indirect, this suggests that the difference is due to the pressure–velocity correlations: that is, the higher values of C_{s1} and C_{s2} are required in order to account for the additional transport due to gradients of $\langle p'u_i\rangle$. There seems to be little merit, therefore, in using elaborate models for the triple correlation when there is an unknown, but comparable, contribution from the pressure–velocity correlations. The simple model of Shir, with $C_{s1} \approx 0.09$. may behave as well as the more complicated suggestions and its simplicity greatly facilitates the solution of the equations.

To conclude: the Reynolds-stress equation is a balance between convection, production, dissipation, turbulent transport and redistribution by the pressure–rate of strain term. The first three of these processes are known. Lumley & Newman's expression for the first part of the redistribution appears most accurate while, for the second part, there is no evidence to warrant going beyond the linear model of Launder, Reece & Rodi. Because of the unknown contribution of the pressure–velocity correlation, the simplest model of turbulent transport, equation (5.13), may behave as well as the more elaborate models for the triple correlations alone.

6. *The dissipation equation*

The rate of dissipation ϵ, which appears in the Reynolds-stress equation, can be determined from its own modelled transport equation. This equation has the form,

$$\rho\frac{\partial\epsilon}{\partial t}+\rho\langle U_i\rangle\frac{\partial\epsilon}{\partial x_i}=\frac{\partial T_i}{\partial x_i}+S_\epsilon, \tag{6.1}$$

where S_ϵ is the net rate of production of ϵ, and T_i is the turbulent transport.

The definition

$$\epsilon\equiv\frac{\mu}{\rho}\left\langle\left(\frac{\partial u_i}{\partial x_j}\right)^2\right\rangle, \tag{6.2}$$

shows that the dissipation of turbulence energy is due to viscous action. However, this is not the rate-controlling process: in a high Reynolds number flow, ϵ is found to be at most a weak function of μ. Rather, ϵ is determined by the rate at which energy is transferred to the smallest scales, and this is an inertial process. That the rate of mixing is governed by inertial processes is especially important in reactive flows, since it allows the assumption (made in §2) that the details of the molecular processes are of secondary importance.

The transport equation for ϵ can be derived from the velocity equation, and hence expressions for T_i and S_ϵ can be obtained. However, these expressions give no guide to the modelling, since they pertain to the viscous processes rather than to the rate-controlling, inertial processes. As a consequence, the modelling of T_i and S_ϵ relies almost entirely on empiricism.

Of the two terms, S_ϵ is the more important and Pope (1976*a*) attempted to justify its modelling in terms of the known quantities $\langle u_i u_j\rangle$, ϵ and $\partial\langle U_i\rangle/\partial x_j$. Justification was provided for flows such as jets, mixing layers and far wakes, but not for rapidly changing flows, such as near wakes. While lack of justification does not constitute condemnation, the physical arguments suggested that this level of closure may prove inadequate in these rapidly changing flows.

In the simple case of the decay of homogeneous isotropic turbulence, the modelled form of S_ϵ can only be

$$S_\epsilon = -C_{\epsilon 2}\rho\epsilon^2/k. \tag{6.3}$$

Lumley & Newman (1977) take $C_{\epsilon 2} = 1.89$ from the data of Comte-Bellot & Corrsin (1966) while Launder, Reece & Rodi (1975) use Batchelor & Townsend's (1948) data to obtain $C_{\epsilon 2} = 1.90$. For the general case, Launder, Reece & Rodi propose

$$S_\epsilon = (\rho\epsilon^2/k)\,(1.44P/\rho\epsilon - 1.90), \tag{6.4}$$

Lumley (1975*a*) gives

$$S_\epsilon = (\rho\epsilon^2/k)\,(0.5P/\rho\epsilon + 12.7\Pi/(1+6\Pi^{\frac{1}{2}}) - 1.865), \tag{6.5}$$

and, for flows without shear, Lumley & Newman give

$$S_\epsilon = (\rho\epsilon^2/k)\,(0.165\ln(1+110\Pi) - 1.89). \tag{6.6}$$

Data of the decay of anisotropic turbulence without shear indicate a dependence upon the anisotropy invariant Π and so, to this extent, (6.5) and (6.6) are to be preferred. In flows with significant shear, however, values of $P/\rho\epsilon$ and Π are closely related, resulting in similar values of S_ϵ being given by (6.4) and (6.5).

There is no direct experimental evidence, nor is there likely to be, to support the modelling of S_ϵ by (6.4) or (6.5) in flows with shear. Further, in general, S_ϵ may be a function of the three invariants of $\langle u_i u_j\rangle$, the five invariants of the velocity gradients and many more invariants involving both $\langle u_i u_j\rangle$ and $\partial\langle U_i\rangle/dx_j$. There can be no direct evidence of the influence of any of the velocity gradient invariants on S_ϵ, and to postulate some dependence based on indirect evidence tends to be speculative. However, one such speculation is of use in the context of jet flames. It is found that the model of Launder, Reece & Rodi, which calculates the properties of most simple flows quite accurately, over estimates the spreading rate of the round jet by about 40 %. Pope (1978) argued that an additional contribution to S_ϵ can be expected when the mean vorticity field is strained. With the appropriate extra term, the model then gives the correct spreading rate for the round jet while its performance in plane flows is unaffected.

The transport term, T_i, remains to be modelled. Various authors have suggested various forms of gradient diffusion, but there is no evidence that complicated suggestions have any advantage over the simplest form; namely

$$T_i = (C_\epsilon \rho k^2/\epsilon)\,\partial\epsilon/\partial x_i, \tag{6.7}$$

where $C_\epsilon \approx 0.07$.

7. *Scalar equations*

For constant-property flows, the transport equations for the mean values of the scalars $\langle\phi_\alpha\rangle$ and the variances $\langle\phi'_\alpha\phi'_\beta\rangle$ are:

$$\rho\frac{\mathrm{D}\langle\phi_\alpha\rangle}{\mathrm{D}t} = \frac{\partial}{\partial x_i}\Gamma\frac{\partial\langle\phi_\alpha\rangle}{\partial x_i} - \frac{\partial\rho\langle u_i\phi'_\alpha\rangle}{\partial x_i} + \rho\langle S_\alpha(\phi)\rangle, \tag{7.1}$$

and

$$\begin{aligned}\rho\frac{\mathrm{D}\langle\phi'_\alpha\phi'_\beta\rangle}{\mathrm{D}t} = {}& \frac{\partial}{\partial x_i}\Gamma\frac{\partial\langle\phi'_\alpha\phi'_\beta\rangle}{\partial x_i} - \frac{\partial\rho\langle u_i\phi'_\alpha\phi'_\beta\rangle}{\partial x_i} + \rho\langle\phi'_\alpha S_\beta(\phi)\rangle + \rho\langle\phi'_\beta S_\alpha(\phi)\rangle \\ & - \rho\langle u_i\phi'_\alpha\rangle\frac{\partial\langle\phi_\beta\rangle}{\partial x_i} - \rho\langle u_i\phi'_\beta\rangle\frac{\partial\langle\phi_\alpha\rangle}{\partial x_i} - 2\Gamma\left\langle\frac{\partial\phi'_\alpha}{\partial x_i}\frac{\partial\phi'_\beta}{\partial x_i}\right\rangle.\end{aligned} \tag{7.2}$$

In equation (7.1), the first term on the right hand side represents transport by molecular diffusion and is negligible at high Reynolds number. The second term, being the gradient of the turbulent scalar flux $\langle u_i \phi'_\alpha \rangle$, represents turbulent transport; and, as has been mentioned, the final term is to be determined from $p(\psi)$. The two scalar flux – mean scalar gradient terms represent the production of $\langle \phi'_\alpha \phi'_\beta \rangle$ due to inhomogeneities in $\langle \phi \rangle$; and

$$\epsilon_{\alpha\beta} = \frac{2\Gamma}{\rho}\left\langle \frac{\partial \phi'_\alpha}{\partial x_i}\frac{\partial \phi'_\beta}{\partial x_i} \right\rangle, \tag{7.3}$$

is the dissipation of $\langle \phi'_\alpha \phi'_\beta \rangle$ due to molecular action. Thus, with the function of S being determined from $p(\psi)$, the remaining unknowns in these equations are $\langle u_i \phi'_\alpha \rangle$, $\langle u_i \phi'_\alpha \phi'_\beta \rangle$ and $\epsilon_{\alpha\beta}$.

Since the scalar flux makes an important appearance in both equations, its determination is considered first. The simplest method, and that used in most flame calculations, is to assume gradient diffusion, giving

$$\langle u_i \phi'_\alpha \rangle = -(C_\phi k^2/\epsilon)\, \partial \langle \phi_\alpha \rangle / \partial x_i, \tag{7.4}$$

An underlying assumption of mixing-length theory (on which equation (7.4) is based) is that the value of the transported quantity (ϕ_α) does not change during the transport process. For reactive scalars, this assumption is unfounded and hence the use of equation (7.4) is dubious. Consequently, the alternative of determining the scalar fluxes from modelled transport equations is preferable.

Ignoring terms that are negligible at high Reynolds number, the transport equation for the scalar flux is

$$\rho \frac{D\langle u_i \phi'_\alpha \rangle}{Dt} = -\frac{\partial \rho \langle u_i u_j \phi'_\alpha \rangle}{\partial x_j} - \rho \langle u_i u_j \rangle \frac{\partial \langle \phi_\alpha \rangle}{\partial x_j} - \rho \langle u_j \phi'_\alpha \rangle \frac{\partial \langle U_i \rangle}{\partial x_j} - \left\langle \phi'_\alpha \frac{\partial p'}{\partial x_i} \right\rangle + \rho \langle u_i S_\alpha(\phi) \rangle. \tag{7.5}$$

This equation has been studied mainly in the context of atmospheric boundary layers with $S_\alpha(\phi)$ equal to zero. In that instance, the principal unknown is $\langle \phi'_\alpha \partial p'/\partial x_i \rangle$, which can be treated in an analogous way to the pressure–rate of strain. Thus, the term can be decomposed as

$$\left\langle \phi'_\alpha \frac{\partial p'}{\partial x_i} \right\rangle = \frac{\partial \langle \phi'_\alpha p' \rangle}{\partial x_i} - \left\langle p'_1 \frac{\partial \phi'_\alpha}{\partial x_i} \right\rangle - \left\langle p'_2 \frac{\partial \phi'_\alpha}{\partial x_i} \right\rangle. \tag{7.6}$$

The first term contributes to transport: the remaining two terms represent the two parts of the pressure–scalar gradient correlation. For the first part, Monin (1965) has suggested the model

$$\langle p'_1 \partial \phi'_\alpha / \partial x_i \rangle = -(C_{\phi 1} \rho \epsilon / k) \langle u_i \phi'_\alpha \rangle. \tag{7.7}$$

(Launder (1976) suggests $C_{\phi 1} = 3.8$.) Assuming that the second part is a linear function of scalar fluxes and velocity gradients, Launder (1973) and Lumley (1975*a*) obtained

$$\left\langle p'_2 \frac{\partial \phi'_\alpha}{\partial x_i} \right\rangle = \tfrac{4}{5} \rho \langle u_j \phi'_\alpha \rangle \frac{\partial \langle U_i \rangle}{\partial x_j} + \tfrac{1}{5} \rho \langle u_j \phi'_\alpha \rangle \frac{\partial \langle U_j \rangle}{\partial x_i}. \tag{7.8}$$

There is no reason to doubt the specific form of (7.8) nor data to support it. On the other hand, Lumley (1975*a*) has proposed a more elaborate expression for $\langle p'_1 \partial \phi'_\alpha / \partial x_i \rangle$ but, as Launder (1976) points out, the only other form for which values of the constants have been suggested is

$$\langle p'_1 \partial \phi'_\alpha / \partial x_i \rangle = -(C_{\phi 1} \rho \epsilon / k) \langle u_i \phi'_\alpha \rangle - (C'_{\phi 1} \rho \epsilon a_{ij} / k) \langle u_j \phi'_\alpha \rangle. \tag{7.9}$$

The scalar flux is itself transported by three mechanisms; turbulent convection, $\langle u_i u_j \phi'_\alpha \rangle$, pressure diffusion, $\langle \phi'_\alpha p' \rangle \delta_{ij}$, and an unknown contribution from $\langle p'_1 \partial \phi'_\alpha / \partial x_i \rangle$. Several models for

$\langle u_i u_j \phi'_\alpha \rangle$ have been suggested (see Launder 1976) but there seems little merit in going beyond the simplest form:

$$\text{transport of } \langle u_i \phi'_\alpha \rangle = \frac{\partial}{\partial x_j} (C_\phi k^2/\epsilon) \frac{\partial \langle u_i \phi'_\alpha \rangle}{\partial x_j}. \tag{7.10}$$

For inert flows, to which the scalar-flux equation is usually applied, this completes the closure but for reacting flows the addition term $\langle u_i S_\alpha(\boldsymbol{\phi}) \rangle$ appears and must be modelled. Because the term is a correlation of S_α with the fluctuating velocity, it cannot be determined from $p(\boldsymbol{\psi})$; a knowledge of $\langle p'(\boldsymbol{\psi})\, u_i \rangle$ is required. In § 11 the modelling of $\langle p'(\boldsymbol{\psi})\, u_i \rangle$ is discussed and it is suggested that a mixing length type of model may be a fair approximation. However, at this level of closure this leads to an inconsistency since $\langle u_i \phi'_\alpha \rangle$ given by the mixing-length model and the value given by the scalar-flux equation are not likely to be the same. In order to avoid the inconsistency the following model is tentatively proposed:

$$\langle p'(\boldsymbol{\psi})\, u_i \rangle = -(C_\phi k^2/\epsilon)\,(\partial p(\boldsymbol{\psi})/\partial x_i) + [u_i/\phi'_\alpha]\,(\psi_\alpha - \langle \phi_\alpha \rangle)\, p(\boldsymbol{\psi}), \tag{7.11}$$

where $C_\phi \approx 0.13$ and $[u_i/\phi'_\alpha]$ is symbolic for

$$[u_i/\phi'_\alpha] = \langle \phi'_\alpha \phi'_\beta \rangle^{-1} (\langle u_i \phi'_\beta \rangle + (C_\phi k^2/\epsilon)\, \partial \langle \phi_\beta \rangle / \partial x_i). \tag{7.12}$$

Summation is implied over repeated suffices. (The significance of the additional term is discussed in § 11.) A model for $\langle u_i S_\alpha(\boldsymbol{\phi}) \rangle$ is obtained by multiplying equation (7.11) by $S_\alpha(\boldsymbol{\psi})$ and integrating:

$$\langle u_i S_\alpha(\boldsymbol{\phi}) \rangle = -(C_\phi k^2/\epsilon)\, \partial \langle S_\alpha(\boldsymbol{\phi}) \rangle / \partial x_i + [u_i/\phi'_\beta]\, \langle \phi'_\beta S_\alpha(\boldsymbol{\phi}) \rangle. \tag{7.13}$$

The correlation $\langle u_i \phi'_\alpha \phi'_\beta \rangle$ which appears in the transport equation for $\langle \phi'_\alpha \phi'_\beta \rangle$ can also be obtained from equation (7.11);

$$\langle u_i \phi'_\alpha \phi'_\beta \rangle = -(C_\phi k^2/\epsilon)\, \partial \langle \phi'_\alpha \phi'_\beta \rangle / \partial x_i + [u_i/\phi'_\gamma]\, \langle \phi'_\alpha \phi'_\beta \phi'_\gamma \rangle. \tag{7.14}$$

Attention is turned to the scalar dissipation $\epsilon_{\alpha\beta}$ and the dissipation of fluctuations of a single scalar is considered first. With $\phi = \phi_\alpha$ and $\epsilon_\phi = \frac{1}{2}\epsilon_{\alpha\alpha}$ (no summation) the transport equation for $\langle \phi'^2 \rangle$ is

$$\rho \mathrm{D} \tfrac{1}{2} \langle \phi'^2 \rangle / \mathrm{D}t = -\rho \langle u_i \phi' \rangle\, \partial \langle \phi \rangle / \partial x_i - \partial \tfrac{1}{2} \rho \langle u_i \phi'^2 \rangle / \partial x_i - \rho \epsilon_\phi. \tag{7.15}$$

The simplest model for ϵ_ϕ is

$$\epsilon_\phi = C_{\phi 2}\, \epsilon \langle \phi'^2 \rangle / \langle u_i^2 \rangle, \tag{7.16}$$

which, in effect, assumes that the time scale of decay of scalar fluctuations is proportional to the decay time scale of velocity fluctuations: $C_{\phi 2}$ is the constant of proportionality. For shear flows in which the scalar and velocity fields share a common history and common boundary conditions, this assumption appears to be satisfactory. Béguier, Dekeyser & Launder (1978) deduced the value of $C_{\phi 2}$ from data of three shear flows: a boundary layer, pipe flow and a plane wake; the value $C_{\phi 2} = 2.0$ fits the data to within 20 % over nearly all of the flows. In addition, Spalding (1971) and Samaraweera (1978), using models incorporating equation (7.16) with $C_{\phi 2} = 2.0$, obtained good agreement with experimental data for round and plane jets, wakes and mixing layers.

These findings support the contention that $C_{\phi 2}$ can be taken as a constant in the type of shear flows mentioned, but there is equally clear evidence that $C_{\phi 2}$ is not a universal constant. Data of the decay of temperature fluctuations in grid generated turbulence (Lin & Lin 1973) show a large spread in decay rates although Launder (1976) suggests $C_{\phi 2} \approx 1.0$ provides a reasonable fit. In other flows values of $C_{\phi 2}$ of 1.25 (Launder 1976) and of 1.4 (Wyngaard 1975) have been used.

In general, then, an alternative method for determining ϵ_ϕ would be preferable. The natural alternative is to solve a separate transport equation for ϵ_ϕ. Such a modelled equation would contain a source $S_{\epsilon\phi}$ of the form

$$S_{\epsilon\phi} = (\rho\epsilon\epsilon_\phi/k)\, F[(k/\epsilon)\,\partial\langle U_i\rangle/\partial x_j, a_{ij}, \langle\phi'^2\rangle\,\epsilon/(k\epsilon_\phi), \quad (k^{\frac{3}{2}}/\epsilon\langle\phi'^2\rangle^{\frac{1}{2}})\,\partial\langle\phi\rangle/\partial x_i], \tag{7.17}$$

where F is an unknown, dimensionless, invariant function. As has been observed by Launder (1976), the task of determining $S_{\epsilon\phi}$ is similar to that of determining S_ϵ except that twice as many quantities are involved, and, it may be added, there is less than half the quantity of relevant experimental data. Consequently, although modelled equations for $S_{\epsilon\phi}$ have been proposed (Lumley & Khajeh-Nouri 1974), there is no evidence that they are more reliable than the simpler equation (7.16).

The form of (7.17) corresponding to a transport equation for $\epsilon_{\alpha\beta}$ is yet more complicated and so, for the moment, a model akin to equation (7.16) seems appropriate. The only admissible model in terms of k, ϵ and $\langle\phi'_\alpha\,\phi'_\beta\rangle$ is

$$\epsilon_{\alpha\beta} = C_{\phi 2}\langle\phi'_\alpha\,\phi'_\beta\rangle\,\epsilon/k. \tag{7.18}$$

Transformation laws (see § 10) exclude other possibilities.

8. *Effects of variable density*

The second order closures of §§ 5–7 have been developed primarily for constant-density flows. Several authors, Lumley (1975*a*) and Launder (1976) for example, have also made allowance for the effects of buoyancy caused by small density variations. The buoyancy forces may be large but, it is assumed, the density variations are small enough for other effects to be negligible. Such an assumption is untenable for flames where, typically, the density varies by a factor of five.

The behaviour of statistical equations in variable-density flows may differ from that of their constant-density counterparts because of the appearance of addition terms, and because existing terms behave differently. Without density weighting, addition terms arise involving fluctuating density correlations: equation (3.8) is an example. On the other hand, it may be seen that the density-weighted equations derived in the appendix appear the same whether the density varies or not. There is no term that vanishes for constant density flows. This indicates that, as written, no additional terms appear, but it does not imply that the terms behave in the same way with and without density variations.

Taking the pressure–rate of strain correlation as an example, it appears that variable density may have an effect. A Poisson equation for pressure can be obtained by taking the divergence of the momentum equation, equation (2.13):

$$\nabla^2 p = -\frac{\partial^2 \rho U_i U_j}{\partial x_i\,\partial x_j} + g_j\frac{\partial\rho}{\partial x_j} + \frac{\partial^2\rho}{\partial t^2} + 2\mu\nabla^2\frac{\partial U_i}{\partial x_i}, \tag{8.1}$$

and from Green's Theorem (neglecting a surface integral), the velocity–pressure gradient correlation is

$$\left\langle u''_k\frac{\partial p}{\partial x_j}\right\rangle = \frac{1}{4\pi}\int\frac{\partial}{\partial r_j}\langle u''_k\,\nabla^2_r p(\boldsymbol{x}+\boldsymbol{r})\rangle\frac{\mathrm{d}\boldsymbol{r}}{|r|}. \tag{8.2}$$

In constant-density flows, all but the leading term in equation (8.1) are zero, giving

$$\begin{aligned}\langle u''_k\,\nabla^2_r p(\boldsymbol{x}+\boldsymbol{r})\rangle &= -\rho\left\langle u_k\frac{\partial^2}{\partial r_i\,\partial r_j}U_i(\boldsymbol{x}+\boldsymbol{r})\,U_j(\boldsymbol{x}+\boldsymbol{r})\right\rangle \\ &= -\rho\frac{\partial^2}{\partial r_i\,\partial r_j}\langle u_k u_i(\boldsymbol{x}+\boldsymbol{r})\,u_j(\boldsymbol{x}+\boldsymbol{r})\rangle - 2\rho\frac{\partial\langle U_i\rangle}{\partial x_j}\frac{\partial}{\partial r_i}\langle u_k u_j(\boldsymbol{x}+\boldsymbol{r})\rangle.\end{aligned} \tag{8.3}$$

It is this analysis that leads to the conclusion that there are two parts to the pressure–rate of strain and guides the modelling. For variable-density flows all the terms in (8.1) are non-zero and even the first term cannot be expressed as simply as (8.3). This demonstrates that the term $\langle u_k'' \partial p/\partial x_j \rangle$ may behave differently in constant-density and variable-density flows.

It is not difficult to suggest how the modelling of the pressure–rate of strain term could be extended to account for variable density; the following could be added:

$$C_1 \left(\frac{\partial \langle \rho \rangle}{\partial x_l}\right)^2 \delta_{ij}, \quad C_2 \frac{\partial \tilde{U}_l}{\partial x_l} \delta_{ij}, \quad C_3 \frac{\partial \langle \rho \rangle}{\partial x_i} \frac{\partial \langle \rho \rangle}{\partial x_j} \quad \text{and} \quad C_4 \frac{\partial^2 \langle \rho \rangle}{\partial x_i \, \partial x_j},$$

as well as linear functions of these terms with the Reynolds stresses and velocity gradients. The difficulty arises in ascribing values to the (supposed) constants. Equation (8.1) is not amenable to analysis, and one cannot expect there to be sufficient experimental data to determine the constants empirically.

The same applies to the dissipation equation: the source of dissipation S_ϵ may be supposed to depend upon $(\partial \langle \rho \rangle / \partial x_i)^2$ and $\partial \tilde{U}_l / \partial x_l$, but there is no means to establish the dependence.

This being the case, the best available hypothesis is that the same modelling applies to the density-weighted equations in variable-density flows as in constant-density flows. There is a shortage of data to test this hypothesis directly but the mixing layer data of Brown & Roshko (1974) provide some evidence. Libby (1973) used a lower-order closure (using density-weighted averaging) to calculate the velocity and density profiles; for one test condition the agreement was very good while, for another, it was less good. There are more data for round jets, but as was mentioned in § 6, standard second-order closures calculate their spreading rates incorrectly even for constant-density flows. In addition, the usefulness of reacting flow data for this purpose is diminished by the uncertainties introduced into the calculations by combustion models. These difficulties are decreasing: laser – Doppler anemometry is providing accurate turbulence data in reactive and non-reactive flows; the modification to the dissipation equation proposed by Pope (1978) allows round jets to be calculated, and, hopefully, the uncertainties in combustion models are lessening.

In comparing measured and calculated values, it is important to compare like with like. Laser–Doppler anemometers measure unweighted quantities whereas those obtained by gas sampling techniques are density-weighted: the precise nature of the quantities measured by other techniques is less certain. There are enough experimental difficulties as it is without demanding that a particular form of averaged quantity be measured. To determine unweighted quantities from calculated density-weighted quantities is comparatively simple. The unweighted joint p.d.f. $p(\psi)$ is related to the density-weighted p.d.f. $\tilde{p}(\psi)$ by

$$\langle \rho \rangle \tilde{p}(\psi) = \rho(\psi) p(\psi), \tag{8.4}$$

and so the unweighted mean of any quantity $f(\phi)$ is given by

$$\langle f(\phi) \rangle = \int p(\psi) f(\psi) \, \mathrm{d}\psi = \int \tilde{p}(\psi) \frac{\langle \rho \rangle}{\rho(\psi)} f(\psi) \, \mathrm{d}\psi. \tag{8.5}$$

The relation between weighted and unweighted velocities is readily determined from their definitions:

$$U_i = \langle U_i \rangle + u_i = \tilde{U}_i + u_i''; \tag{8.6}$$

therefore

$$\langle U_i \rangle = \tilde{U}_i + \langle u_i'' \rangle, \tag{8.7}$$

and thus

$$u_i = u_i'' - \langle u_i'' \rangle. \tag{8.8}$$

From these equations, the unweighted velocity and Reynolds stresses are seen to be

$$\langle U_i \rangle = \tilde{U}_i + \langle u_i'' \rangle, \tag{8.9}$$

and

$$\langle u_i u_j \rangle = \widetilde{u_i'' u_j''} + \langle u_i'' \rangle \langle u_j'' \rangle - \langle \rho' u_i u_j \rangle / \langle \rho \rangle. \tag{8.10}$$

The final term in (8.10) can be assumed to be small, since, to a first approximation,

$$\langle \rho' u_i u_j \rangle \approx \langle \rho' \rangle \langle u_i u_j \rangle + \langle \rho' u_i \rangle \langle u_j \rangle + \langle \rho' u_j \rangle \langle u_i \rangle = 0. \tag{8.11}$$

Thus, a knowledge of $\langle u_i'' \rangle$ is all that is required to determine $\langle U_i \rangle$ and $\langle u_i u_j \rangle$. $\langle u_i'' \rangle$ can be expressed as

$$\langle u_i'' \rangle = \langle \rho \rangle \widetilde{u_i''/\rho} = \langle \rho \rangle \int \frac{\widetilde{u_i'' p'(\psi)}}{\rho(\psi)} \, \mathrm{d}\psi. \tag{8.12}$$

A consistent model can be obtained by using the density-weighted equivalent of the model for $\langle p'(\psi) u_i \rangle$, equations (7.11) and (7.12). This leads to

$$\langle u_i'' \rangle = C_\phi \frac{\tilde{k}^2}{\tilde{\epsilon}} \frac{1}{\langle \rho \rangle} \frac{\partial \langle \rho \rangle}{\partial x_i} + [u_i''/\phi_\alpha''] \, (\langle \phi_\alpha \rangle - \tilde{\phi}_\alpha), \tag{8.13}$$

where $[u_i''/\phi_\alpha'']$ is the density-weighted form of $[u_i/\phi_\alpha']$ (equation 7.12).

Thus, unweighted mean values of scalars can be determined, without approximation, from equation (8.5) and the unweighted velocities and Reynolds stresses can be determined from equations (8.9), (8.10) and (8.13).

9. *Assessment of models*

We should like to answer the following questions: For what types of flow are second order closures adequate? And, for such flows, are the specific models introduced in the previous sections accurate? It is important to distinguish between these questions and to realize that they must be answered in different ways.

The first question is of greater lasting significance but no satisfactory answer has been provided. Attempts tend to be disappointing. As an illustration, modelling the pressure–rate of strain term can be justified for homogeneous turbulence and first order departures from it. But, without quantifying the inaccuracy caused by departures from homogeneity, the result is of limited value. Similarly, modelling of the source in the dissipation equation, S_ϵ, can be justified provided that the normalized Reynolds stresses and velocity gradients are nearly homogeneous and that the normalizing parameters, k and ϵ say, change at a nearly constant rate (Pope 1976*a*). In other words, second order closures are adequate for nearly-homogeneous, near-equilibrium flows and can be expected to become progressively inaccurate for departures from these conditions. The unanswered question is: how inaccurate? Nevertheless, with little uncertainty, it can be concluded that this level of closure is adequate for free shear flows – jets, wakes and mixing layers – but for rapidly changing flows, such as those with recirculation, the question is undecided.

The second question – are the specific models accurate? – can be answered by comparing solutions of the model equations with experimental data. The model of Launder, Reece & Rodi (1975) has been tested in jets, wakes and mixing layers by themselves, by Pope & Whitelaw (1976), and by Samaraweera (1978). Except for the spreading rate of the round jet, the agreement between calculations and experiment is good. Typically, mean quantities are in error by less than 5 % and turbulence quantities by less than 20 %. In addition, Samaraweera obtained similar agreement for a passive scalar, the scalar flux and the scalar variance. There are, however, discrepancies in the round jet, the round jet with swirl (Launder & Morse 1977) and recirculating flows (Pope & Whitelaw 1976). It is likely, at least in the first two cases, that the discrepancy is due to inaccuracy in the modelling, not to the inadequacy of the level of closure. In future attempts to increase the accuracy of the model, the proposals of Lumley & Newman (1977) and of Pope (1978) should prove useful.

Less can be said about the accuracy of the scalar equations because they have not been comprehensively tested. The work of Samaraweera (1978) is encouraging, as it shows accurate calculations for three free shear flows. There are also several works related to atmospheric boundary layers in which modelled scalar equations are solved (see Launder 1976 for references). However, these flows are dominated by wall effects and, in many cases, by buoyancy. Consequently they are less relevant to the present purpose. The available data are sufficient for testing the model equations for $\langle u_i \phi'_\alpha \rangle$ and $\langle \phi'_\alpha \phi'_\alpha \rangle$ (no summation) in inert, constant-density flows. But it is unlikely that measurements of $\langle \phi'_\alpha \phi'_\beta \rangle$ $(\alpha \neq \beta)$ in inert flows or of any of those quantities in reactive flows will be available for some time. In summary: a more precise assessment of the modelled scalar equations must await further testing: data are available for this purpose.

C. PROBABILITY DISTRIBUTIONS

10. *Definitions and properties*

In the theoretical description of turbulent flames, the usefulness of the joint probability function stems from the fundamental property density

$$\langle Q(\boldsymbol{\phi}(\boldsymbol{x},t))\rangle = \int p(\boldsymbol{\psi};\, \boldsymbol{x},t)\, Q(\boldsymbol{\psi})\, \mathrm{d}\boldsymbol{\psi}. \tag{10.1}$$

That is, for any function Q – a reaction rate for example – the ensemble average can be determined from $p(\boldsymbol{\psi})$. In this section some of the properties of $p(\boldsymbol{\psi})$ are presented. The next section is concerned with the transport equation for $p(\boldsymbol{\psi})$. This equation is useful in describing the physical behaviour of $p(\boldsymbol{\psi})$, but its solution in modelled form is only feasible for the simplest of cases. A practical means of determining $p(\boldsymbol{\psi})$ is to assume that, in a turbulent flame, $p(\boldsymbol{\psi})$ is the statistically most likely distribution. The method of determining this distribution is presented in § 12.

The joint p.d.f. of a set of scalars – $\phi_\alpha(\boldsymbol{x},t)$, $\alpha = 1, 2, \ldots, \sigma$ – is defined such that $p(\boldsymbol{\psi};\, \boldsymbol{x},t)\, \mathrm{d}\boldsymbol{\psi}$ is the probability that $\boldsymbol{\phi}$ lies in the interval

$$\boldsymbol{\psi} < \boldsymbol{\phi}(\boldsymbol{x},t) < \boldsymbol{\psi} + \mathrm{d}\boldsymbol{\psi}. \tag{10.2}$$

$\mathrm{d}\boldsymbol{\psi} = \mathrm{d}\psi_1\, \mathrm{d}\psi_2 \ldots \mathrm{d}\psi_\sigma$ represents an elemental hypervolume at $\boldsymbol{\psi}$. Equation (10.1) follows from this definition and from the definition of an ensemble average. Henceforth, $p(\boldsymbol{\psi};\, \boldsymbol{x},t)$ is written $p(\boldsymbol{\psi})$, the dependence upon $\boldsymbol{x}$ and t being implied.

$p(\boldsymbol{\psi})$ can be related to $\boldsymbol{\phi}(\boldsymbol{x},t)$ in terms of Dirac delta functions. Defining

$$\delta(\boldsymbol{\phi}(\boldsymbol{x},t) - \boldsymbol{\eta}) \equiv \prod_{\alpha=1}^{\sigma} \delta(\phi_\alpha(\boldsymbol{x},t) - \eta_\alpha), \tag{10.3}$$

and substitution of this for Q in equation (10.1) produces

$$\langle \delta(\boldsymbol{\phi}(\boldsymbol{x},t) - \boldsymbol{\eta})\rangle = \int p(\boldsymbol{\psi})\, \delta(\boldsymbol{\psi} - \boldsymbol{\eta})\, \mathrm{d}\boldsymbol{\psi}. \tag{10.4}$$

The right hand side is nothing but $p(\boldsymbol{\eta})$, and so (changing $\boldsymbol{\eta}$ to $\boldsymbol{\psi}$) $p(\boldsymbol{\psi})$ is given by

$$p(\boldsymbol{\psi}) = \langle \delta(\boldsymbol{\phi}(\boldsymbol{x},t) - \boldsymbol{\psi})\rangle. \tag{10.5}$$

It is also possible to take this relation as the definition of $p(\psi)$. Equation (10.1) can then be recovered by multiplying by $Q(\psi)$ and integrating. The transport equation for $p(\psi)$ (considered in the next section) can be deduced from equation (10.5).

The density-weighted joint p.d.f. is defined by

$$\tilde{p}(\psi) = p(\psi)\,\rho(\psi)/\langle\rho\rangle. \tag{10.6}$$

Multiplying by $Q(\psi)$ and integrating yields

$$\int \tilde{p}(\psi)\, Q(\psi)\, \mathrm{d}\psi = \tilde{Q}(\psi). \tag{10.7}$$

Thus, density-weighted averages can be obtained directly from $\tilde{p}(\psi)$.

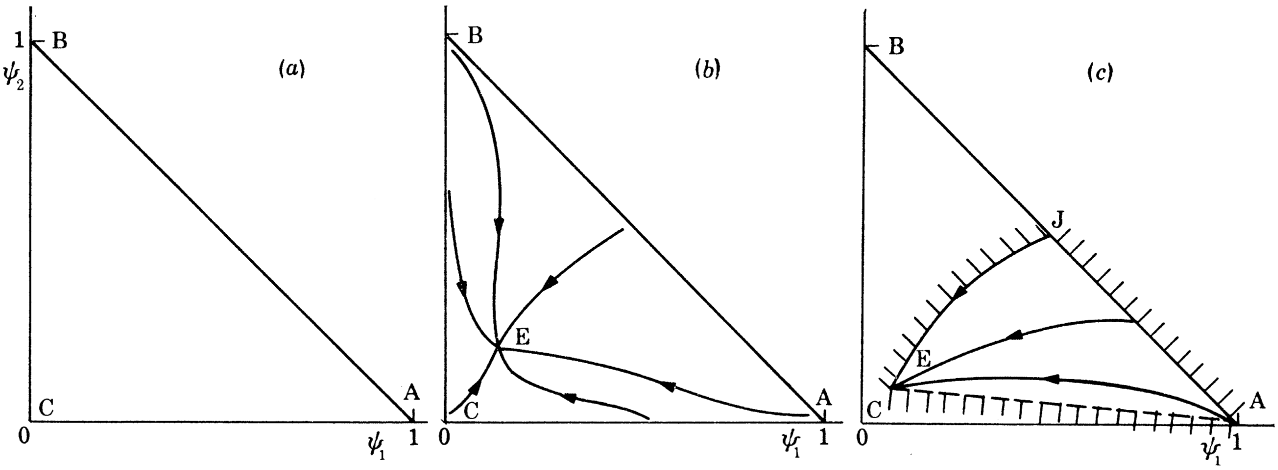

FIGURE 2. (a) The (ψ_1, ψ_2) composition space. (b) Reaction paths in the (ψ_1, ψ_2) composition space. (c) The accessible region of a (ψ_1, ψ_2) composition space.

$p(\psi)$ is a distribution in ψ-space. Different locations in ψ-space correspond to different compositions of the gaseous mixture and so ψ is termed the composition space. Some properties of composition spaces are illustrated by reference to the following example. A reaction takes place between species A and species B to form species C, these being the only three compounds involved:

$$\mathrm{A} + \mathrm{B} \rightleftharpoons \mathrm{C}. \tag{10.8}$$

Then, with $\phi_1 \equiv m_{\mathrm{A}}$ and $\phi_2 \equiv m_{\mathrm{B}}$, since the mass fractions sum to unity, m_{C} is given by

$$m_{\mathrm{C}} = 1 - \phi_1 - \phi_2. \tag{10.9}$$

The (ψ_1, ψ_2) composition space is sketched in figure 2a. The locations (1, 0), (0, 1) and (0, 0) correspond respectively to pure A, pure B and pure C. The lines joining any two of these points correspond to a mixture of two components in the absence of the third, while within the triangle all three species exist. Locations outside the triangle correspond to a negative mass fraction for at least one species: such a composition cannot occur. In general, the region of a composition space that corresponds to compositions that cannot occur is termed the *disallowed region*. The remainder of the space is the *allowed region*. In the example, the sides and interior of the triangle ABC comprise the allowed region.

The rates of increase of A and B due to reaction are $S_1(\phi_1, \phi_2)$ and $S_2(\phi_1, \phi_2)$. In general, *reaction paths* in a composition space are defined by

$$\psi = \Psi(y), \tag{10.10}$$

where

$$\mathrm{d}\Psi_\alpha(y)/\mathrm{d}y = S_\alpha(\Psi). \tag{10.11}$$

y is the distance along the path from some arbitrarily chosen starting point, ψ_0. Reaction paths can be interpreted as follows: if, at time t_0, a homogeneous (non-turbulent) gas mixture has composition $\phi = \psi_0$, at time t_0+y the composition is $\phi = \Psi(y)$. That is, the changing compositions follow a reaction path. The *speed along a path* is defined as

$$s(\psi) = (\sum_\alpha S_\alpha^2(\psi))^{\frac{1}{2}}. \tag{10.12}$$

If $s(\psi)$ is zero, a reaction path is not defined. Reaction paths in the (ψ_1, ψ_2) composition space are sketched in figure 2*b*. The essential feature of the sketch is that all paths lead to the point E where the speed is zero. This location corresponds to the composition at chemical equilibrium.

The allowed region, reaction paths and the speed along a path are all functions of the properties of the gas mixture. They do not depend upon the nature of the flow in which the reaction is taking place.

In a given flow, not all of the allowed compositions may be accessible. The *accessible region* of the composition space contains all locations corresponding to compositions that could occur in the flame under consideration. The accessible region depends upon the flow. The following three rules determine the compositions that are accessible: (i) all compositions that are specified as boundary or initial conditions are accessible; (ii) all compositions lying on reaction paths starting from accessible compositions are also accessible compositions; (iii) all compositions lying on a straight line between two accessible compositions are also accessible compositions.

The first rule is obvious: boundary and initial compositions occur and therefore, by definition, are in the accessible region. The second and third refer to reaction and mixing, respectively. If there is no mixing then compositions follow reaction paths; hence, (ii). In order to illustrate rule (iii), consider the mixing of mass a of a gas mixture of composition $\phi = (\psi)_1$ and mass b with $\phi = (\psi)_2$. The result is mass $(a+b)$ of composition $\phi = (\psi(y))_3$, where

$$(\psi(y))_3 = y(\psi)_1 + (1-y)(\psi)_2 \tag{10.13}$$

and $y = a/(a+b)$. $(\psi(y))_3$, it may be seen, is a straight line between $(\psi)_1$ and $(\psi)_2$. Thus, mixing between two accessible compositions can give rise to compositions on the joining straight line: these compositions are also accessible therefore.

From these rules it can be deduced that the accessible region is the smallest convex region which contains all the specified boundary and initial compositions and which, on its boundary, has no outward pointing reaction path.

Returning to the example, for a jet of composition $m_\mathrm{A} = \frac{1}{2}$, $m_\mathrm{B} = \frac{1}{2}$ issuing into an atmosphere of pure A, the accessible region is sketched in figure 2*c*. The boundary compositions are at A and J. Compositions on the straight line AJ and AE can occur as a result of mixing and along the reaction path JE as a result of reaction. Subsequently, any other composition within the region can occur by mixing.

Useful information is obtained by considering the behaviour of $p(\psi)$ and of the composition space when the scalars ϕ are subjected to a linear transformation:

$$\phi_\alpha^* \equiv a_{\alpha\beta}\phi_\beta + b_\alpha. \tag{10.14}$$

The transport equation (2.14) for $\boldsymbol{\phi}$ can be written

$$\mathrm{L}(\phi_\alpha) = S_\alpha(\boldsymbol{\phi}), \tag{10.15}$$

where L is a linear differential operator:

$$\mathrm{L} \equiv \left(\frac{\partial}{\partial t} + U_i \frac{\partial}{\partial x_i} - \frac{1}{\rho}\frac{\partial}{\partial x_i}\Gamma\frac{\partial}{\partial x_i}\right). \tag{10.16}$$

Substituting the definition of ϕ_α^* into the transport equations produces

$$\mathrm{L}(\phi_\alpha^*) = S_\alpha^*(\boldsymbol{\phi}^*), \tag{10.17}$$

where the transformed reaction rate has been defined by

$$S_\alpha^*(\boldsymbol{\phi}^*) \equiv a_{\alpha\beta} S_\beta(\boldsymbol{\phi}).\dagger \tag{10.18}$$

In principle, $\boldsymbol{\phi}^*$ could be determined in two ways: by solving its transport equation; or by solving the transport equation for $\boldsymbol{\phi}$ and then performing the transformation. Clearly, the result obtained by each method is the same. It is equally clear that the theory should also produce results that transform correctly. The modelling of $\epsilon_{\alpha\beta}$ and $\langle u_i\,\phi'_\alpha\rangle$ is §7 is guided by this principle.

The transformation of moments is straightforward. The mean is

$$\langle\phi_\alpha^*\rangle = a_{\alpha\beta}\langle\phi_\beta\rangle + b_\alpha, \tag{10.19}$$

and, writing $C_{\alpha\beta}$ for $\langle\phi'_\alpha\,\phi'_\beta\rangle$ and $C_{\alpha\beta}^*$ for $\langle\phi_\alpha^{*\prime}\phi_\beta^{*\prime}\rangle$, the second moments are

$$C_{\alpha\beta}^* = a_{\alpha\gamma}\,a_{\beta\delta}\,C_{\gamma\delta}. \tag{10.20}$$

The transformed composition space $\boldsymbol{\psi}^*$ is given by

$$\psi_\alpha^* = a_{\alpha\beta}\,\psi_\beta + b_\alpha, \tag{10.21}$$

and the joint p.d.f. of $\boldsymbol{\phi}^*$ is defined such that $p^*(\boldsymbol{\psi}^*)\,\mathrm{d}\boldsymbol{\psi}^*$ is the probability that $\boldsymbol{\phi}^*$ lies in the range $\boldsymbol{\psi}^* < \boldsymbol{\phi}^* < \boldsymbol{\psi}^* + \mathrm{d}\boldsymbol{\psi}^*$. It follows that p and p^* are related by

$$p^*(\boldsymbol{\psi}^*)\,\mathrm{d}\boldsymbol{\psi}^* = p(\boldsymbol{\psi})\,\mathrm{d}\boldsymbol{\psi}, \tag{10.22}$$

or

$$p^*(\boldsymbol{\psi}^*) = p(\boldsymbol{\psi})\,|\partial\boldsymbol{\psi}^*/\partial\boldsymbol{\psi}|^{-1} = p(\boldsymbol{\psi})\,|\boldsymbol{a}|^{-1}. \tag{10.23}$$

Here, $|\partial\boldsymbol{\psi}^*/\partial\boldsymbol{\psi}|$ represents the determinant of the Jacobian of the transformation which is equal to the determinant of $\boldsymbol{a}$. An expression for $|\boldsymbol{a}|$ is obtained by taking the determinant of both sides of equation (10.20):

$$|\boldsymbol{C}^*| = |\boldsymbol{a}|^2\,|\boldsymbol{C}|. \tag{10.24}$$

Thus, the relation between p and p^* can be written

$$|\boldsymbol{C}|^{\frac{1}{2}}p(\boldsymbol{\psi}) = |\boldsymbol{C}^*|^{\frac{1}{2}}p^*(\boldsymbol{\psi}^*). \tag{10.25}$$

$|\boldsymbol{C}|^{\frac{1}{2}}$ has a clear physical interpretation. $C_{\alpha\beta}$ is symmetric and so can be diagonalized by a pure rotation. The determinant (which is unaffected by rotation) is then the product of the diagonal elements which are the squares of the standard deviations in each direction. Thus $|\boldsymbol{C}|^{\frac{1}{2}}$ is the product of these standard deviations: it may be thought of as a normalization for $p(\boldsymbol{\psi})$. Equation (10.25) contains the important result that the normalized joint p.d.f., $|\boldsymbol{C}^*|^{\frac{1}{2}}p^*(\boldsymbol{\psi}^*)$, is invariant under linear transformations. That is, the value of $|\boldsymbol{C}^*|^{\frac{1}{2}}p^*(\boldsymbol{\psi}^*)$ is independent of the transformation parameters $a_{\alpha\beta}$ and b_α.

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† Here and elsewhere summation is implied over repeated indices.

There is one other function of the composition space that is invariant under linear transformations: this is the normalized speed along a path or the *normalized reaction speed* $\Omega(\psi)$,

$$\Omega^2(\psi) = C_{\alpha\beta}^{-1} S_\alpha(\psi) S_\beta(\psi). \tag{10.26}$$

Again, the physical significance of $\Omega(\psi)$ can best be seen in the diagonal frame in which case,

$$\Omega^2(\psi) = \sum_\alpha S_\alpha^2(\psi)/C_{\alpha\alpha}. \tag{10.27}$$

That is, $\Omega(\psi)$ is the Euclidean norm of the reaction rates normalized by the standard deviations.

These transformation laws and the invariant $\Omega(\psi)$ are used in the following sections.

11. *Transport equations*

The p.d.f. transport equation is examined in order to provide an understanding of the processes affecting p.d.fs in reactive flows. The equation provides a description of the transport of $\tilde{p}(\psi)$ in position and composition spaces with the effect of chemical reaction appearing in closed form. To model and solve this equation is a useful research exercise, but it is unlikely that this direct approach will prove to be practicable except in the simplest of cases. Consequently, the modelling is not discussed in great detail.

The transport equation for the density-weighted joint p.d.f. is

$$\langle\rho\rangle \frac{\mathrm{D}\tilde{p}(\psi)}{\mathrm{D}t} + \frac{\partial \langle\rho\rangle \widetilde{u_i'' p'(\psi)}}{\partial x_i} = -\frac{\partial \langle\rho\rangle \tilde{p}(\psi)\, S_\alpha(\psi)}{\partial \psi_\alpha} - \frac{\partial}{\partial \psi_\alpha}\left\langle p'(\psi) \frac{\partial}{\partial x_i} \Gamma \frac{\partial \phi_\alpha}{\partial x_i}\right\rangle, \tag{11.1}$$

where $p'(\psi)$ is written for $\delta(\psi - \phi)$. The terms on the left hand side represent convection by the mean flow and by turbulence; they account for the transport of $\tilde{p}(\psi)$ in position space. The terms on the right hand side account for the transport of $\tilde{p}(\psi)$ in composition space due to reaction and molecular mixing.

The convection of $\tilde{p}(\psi)$ by the mean flow is known in terms of $\tilde{p}(\psi)$ and $\tilde{U}$, while the turbulent convection is due to the correlation $\widetilde{u_i'' p'(\psi)}$. Two models for the similar correlation $\langle u_i p'(\psi)\rangle$ have been proposed: the proposal of Dopazo (1975) can be generalized to

$$\widetilde{u_i'' p'(\psi)} = (\widetilde{\phi_\alpha'' \phi_\beta''})^{-1} \widetilde{\phi_\beta'' u_i''} (\psi_\alpha - \tilde{\phi}_\alpha)\, \tilde{p}(\psi), \tag{11.2}$$

and the gradient diffusion model proposed by Pope (1976*b*) is

$$\widetilde{u_i'' p'(\psi)} = -(C_\phi k^2/\epsilon)\, \partial \tilde{p}(\psi)/\partial x_i. \tag{11.3}$$

Dopazo's proposal is accurate for small departures from Gaussianity and homogeneity. On the other hand, for large departures from these conditions, the gradient diffusion model is likely to be better behaved since it results in an elliptic (rather than a hyperbolic) partial differential equation for $\tilde{p}(\psi)$.

The use of equation (11.3) in conjunction with a second order closure would lead to an inconsistency. This is because the value of $\widetilde{u_i'' \phi_\alpha''}$ obtained from the gradient diffusion model is likely to be different from that given by its transport equation. In order to avoid the inconsistency a correction can be added, giving

$$\widetilde{u_i'' p'(\psi)} = -(C_\phi k^2/\epsilon)\, \partial \tilde{p}(\psi)/\partial x_i + (\widetilde{\phi_\alpha'' \phi_\beta''})^{-1} (\widetilde{\phi_\beta'' u_i''})_{\mathrm{d}} (\psi_\alpha - \tilde{\phi}_\alpha)\, \tilde{p}(\psi), \tag{11.4}$$

where $(\widetilde{\phi_\beta'' u_i''})_{\mathrm{d}}$ is the difference between the scalar flux and its value according to the gradient diffusion model;

$$(\widetilde{\phi_\beta'' u_i''})_{\mathrm{d}} = \widetilde{\phi_\beta'' u_i''} + (C_\phi k^2/\epsilon)\, (\partial \tilde{\phi}_\beta/\partial x_i). \tag{11.5}$$

The additional term is simply Dopazo's model evaluated with the scalar flux difference rather than the scalar flux itself.

The most notable feature of the transport equation for $\tilde{p}(\psi)$ is that the effect of reaction appears in closed form: no term associated with reaction needs to be modelled. In order to interpret the effect of $S_\alpha(\psi)$ upon $\tilde{p}(\psi)$, consider the hypothetical case of the evolution of $\tilde{p}(\psi)$ in homogeneous turbulence without mixing (i.e. $\Gamma = 0$). Equation (11.1) then reduces to

$$\frac{\partial \tilde{p}(\psi)}{\partial t} + \frac{\partial \tilde{p}(\psi)\, S_\alpha(\psi)}{\partial \psi_\alpha} = 0. \tag{11.6}$$

The mathematical interpretation of this simple equation is slightly subtle, but the physical interpretation of the process involved is straightforward. The physical interpretation is given first and then the mathematical justification is provided.

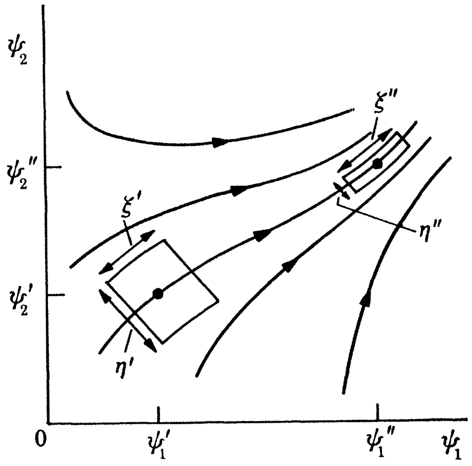

FIGURE 3. Transport of probability in composition space due to reaction.

Reaction paths in the two-dimensional composition space (ψ_1, ψ_2) are sketched in figure 3. At $t = t_0$ the p.d.f. at (ψ_1', ψ_2') is $\tilde{p}(\psi_1', \psi_2'; t_0)$, and the probability within the indicated element is $\tilde{p}(\psi_1', \psi_2'; t_0)\, \eta'\xi'$. As time progresses, the effect of reaction is to transport this element along the reaction path at the speed $s(\psi)$. If $s(\psi)$ is increasing along the path then the element is stretched in the direction of the path. The width of the element normal to the path increases if the paths are diverging and decreases if they are converging. The probability within the element remains constant: thus at time $t = t_1$, when the element is at (ψ_1'', ψ_2''), we have

$$\tilde{p}(\psi_1'', \psi_2''; t_1)\, \eta''\xi'' = \tilde{p}(\psi_1', \psi_2'; t_0)\, \eta'\xi'. \tag{11.7}$$

Such a process should be expressible as a hyperbolic equation with the reaction paths as the characteristics. Indeed this is so; but, as equation (11.7) indicates, the quantity that is conserved along the characteristic is not $\tilde{p}(\psi)$. By defining $\theta(\psi)$ by the equation

$$\partial\{S_\alpha(\psi)/\theta(\psi)\}/\partial\psi_\alpha = 0, \tag{11.8}$$

equation (11.6) can be rewritten as

$$\left(\frac{\partial}{\partial t} + S_\alpha(\psi)\frac{\partial}{\partial \psi_\alpha}\right)(\tilde{p}(\psi; t)\, \theta(\psi)) = 0. \tag{11.9}$$

The reaction paths are characteristics of this equation, which has the solution

$$\tilde{p}(\boldsymbol{\Psi}(t);t)\,\theta(\boldsymbol{\Psi}(t)) = \tilde{p}(\psi_0, t_0)\,\theta(\psi_0). \tag{11.10}$$

It may be seen that $\theta(\boldsymbol{\Psi}(t))$ plays the rôle of $\eta''\xi''$, and that $\theta(\boldsymbol{\Psi}(t))/\theta(\psi_0)$ represents the fractional dilatation of an elemental volume.

Thus, reaction causes probability to be transported along reaction paths at the speed $s(\psi)$. Probability – but not probability density – is conserved in this process.

The final term in the transport equation for $\tilde{p}(\psi)$ represents mixing by molecular action. The evolution of $\tilde{p}(\psi)$ in the absence of all other effects corresponds to the decay of the joint p.d.f. of inert scalars in homogeneous turbulence. The equation then becomes

$$\langle\rho\rangle\frac{\partial\tilde{p}(\psi)}{\partial t} = -\frac{\partial}{\partial\psi_\alpha}\left\langle p'(\psi)\frac{\partial}{\partial x_i}\Gamma\frac{\partial\phi_\alpha}{\partial x_i}\right\rangle = \langle\rho\rangle E(\psi). \tag{11.11}$$

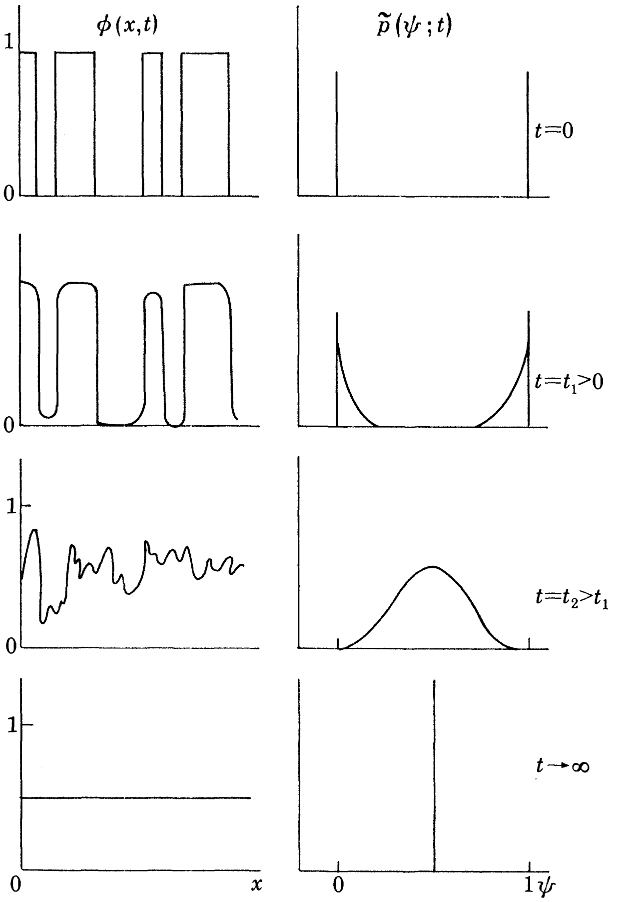

FIGURE 4. The evolution of $\phi(x,t)$ and $\tilde{p}(\psi;t)$ in homogeneous turbulence.

Thus $E(\psi)$ is defined. The modelling of $E(\psi)$ is not straightforward nor has a completely satisfactory model been demonstrated. The aim here is to show the effects that molecular action has on the p.d.f., to show how these effects are reflected in the transport equation, and to give a brief description of the modelling difficulties. The modelling is a specialist activity and until a satisfactory model is developed there is little virtue in describing the models in great detail. However, a brief description is appropriate since the form of such models has implications for the ease of solution of the equations.

The effects of molecular action on p.d.fs is best demonstrated by considering the evolution of $\tilde{p}(\psi)$ in homogeneous turbulence. Consider an initial distribution of two equal delta functions at $\psi = 0$ and $\psi = 1$;

$$\tilde{p}(\psi) = \tfrac{1}{2}\delta(\psi) + \tfrac{1}{2}\delta(1-\psi). \tag{11.12}$$

The evolution of $\tilde{p}(\psi)$ is governed by equation (11.11), the change in time being due solely to molecular action. As the double delta function distribution can only be realized by a rectangular wave-form of $\phi(\boldsymbol{x}, t)$, diffusion will rapidly smooth the discontinuities. This process is sketched in figure 4. The initial rectangular wave and associated double delta function p.d.f. evolve to a smoother waveform and consequently $\tilde{p}(\psi)$ adopts the indicated shape. Eventually diffusion eliminates all fluctuations giving $\phi = \frac{1}{2}$ and thus

$$\tilde{p}(\psi) = \delta(\psi - \tfrac{1}{2}). \tag{11.13}$$

At intermediate times $\tilde{p}(\psi)$ is presumed to adopt the shape indicated on the figure. Intuitively, and as the results of the next section indicate, as $\tilde{p}(\psi)$ tends to a delta function at $\psi = \frac{1}{2}$ it does so as a Gaussian distribution. Consequently not only do all moments tend to zero but so also do the cumulants.

It is important to recognise the effects that molecular action cannot cause. Molecular action cannot alter the mean value of $\tilde{\phi}_\alpha$, it cannot increase the variance $\widetilde{\phi''_{(\alpha)}\phi''_{(\alpha)}}$ (no summation), and it cannot cause $\tilde{p}(\psi)$ to be non-zero outside the accessible region of ψ-space. The influence on the moments can be deduced by expressing equation (11.11) in the form (see Pope 1976*b*)

$$\langle\rho\rangle \frac{\partial \tilde{p}(\psi)}{\partial t} = -\frac{\partial^2}{\partial\psi_\alpha\,\partial\psi_\beta}\left\langle \Gamma p'(\psi)\,\frac{\partial\phi_\alpha}{\partial x_i}\frac{\partial\phi_\beta}{\partial x_i}\right\rangle. \tag{11.14}$$

Integrating this equation to form equations for the moments yields

$$\langle\rho\rangle\,\partial\tilde{\phi}_\alpha/\partial t = 0, \tag{11.15}$$

and

$$\langle\rho\rangle \frac{\partial\widetilde{\phi''_\alpha\phi''_\beta}}{\partial t} = -2\int\left\langle \Gamma p'(\psi)\,\frac{\partial\phi_\alpha}{\partial x_i}\frac{\partial\phi_\beta}{\partial x_i}\right\rangle \mathrm{d}\psi. \tag{11.16}$$

The first equation indicates that $\tilde{\phi}_\alpha$ is unaffected by mixing, and in equation (11.16) with $\alpha = \beta$ the integral is positive indicating that $\widetilde{\phi''_{(\alpha)}\phi''_{(\alpha)}}$ is a decreasing function of time. That mixing cannot cause $\tilde{p}(\psi)$ to become non-zero outside the accessible region was illustrated in the previous section. It can also be shown that this follows from the definition of $E(\psi)$. The lengthy proof of this is not included here since the result is obvious from physical reasoning.

Possibly the first model of the effects of molecular action was the 'conditionally Gaussian' model introduced by Dopazo (see Dopazo 1975). This has the virtue of mathematical simplicity but, unfortunately, it does not produce the correct qualitative behaviour. This point is discussed by Pope (1976*b*, 1979*a*) and by Dopazo (1979*a*, *b*). Pope (1976*b*) considered the modelling of $E(\psi)$ for a single scalar and proposed a model that contained the product of two integrals in ψ-space. This model produces the correct qualitative behaviour but, because of the integrals, it is computationally expensive. Recently Dopazo (1979*a*) and Kollmann (1979) independently suggested models for $E(\psi)$ which are also products of integrals. These three integral models are for a single scalar only. Earlier, but in a different context, Curl (1963) suggested a model for $E(\psi)$ which takes the form of an integral over ψ-space. Again, this produces the correct qualitative behaviour. However, none of the models has been shown to produce the correct quantitative behaviour. For example, none of them shows $\tilde{p}(\psi)$ tending to a delta function as the limit of a Gaussian.

This type of modelling appears to lead to a general expression of the form

$$\tau E(\psi) = \int \tilde{p}(\psi+\psi^*) \int_0^\infty \tilde{p}(\psi-\xi\psi^*)\, g(\psi-\tfrac{1}{2}\psi^*(\xi-1), \psi^*, \xi)\, \mathrm{d}\xi\, \mathrm{d}\psi^*$$

$$-\tilde{p}(\psi) \iint_0^\infty \tilde{p}(\psi-(1+\xi)\,\psi^*)\, g(\psi-\tfrac{1}{2}\psi^*(\xi+1), \psi^*, \xi)\, \mathrm{d}\xi\, \mathrm{d}\psi^*, \quad (11.17)$$

where τ is a turbulent time scale, and the kernel g is positive and an even function of its second argument. We do not wish to go into the details of the model but only to note its form. There are two terms each of which is a volume integral over ψ-space of an integral along a line in ψ-space. To compute this quantity in a composition space of more than one dimension would be a formidable task. It is for this reason that the direct approach of solving a modelled transport equation for $\tilde{p}(\psi)$ is only practicable in simple cases.

To summarize: a transport equation for the density-weighted joint p.d.f. can be deduced from the definition of $\tilde{p}(\psi)$ and from the transport equation for ϕ. $\tilde{p}(\psi)$ is transported in position space by mean flow and turbulent convection and in composition space by reaction and molecular mixing. A consistent model for the turbulent flux $\widetilde{p'(\psi)u''_i}$ has been proposed. The effect of reaction is to transport probability along reaction paths in composition space at the speed $s(\psi)$. Molecular mixing, while not affecting $\tilde{\phi}_\alpha$, tends to reduce the variances $\widetilde{\phi''_{(\alpha)}\phi''_{(\alpha)}}$ and, in the limit, it causes $\tilde{p}(\psi)$ to tend to a delta function (presumably) as the limit of a Gaussian. A completely satisfactory model of the mixing has yet to be demonstrated, but it appears that the complicated form that such a model adopts will restrict the solution of the modelled equation to simple cases.

12. *Assumed distributions*

In a system characterized by σ scalars, the transport equations for $\tilde{\boldsymbol{\phi}}$ contain the mean reaction rates $\tilde{\boldsymbol{S}}(\boldsymbol{\phi})$ which can be determined from the σ-dimensional joint p.d.f. $\tilde{p}(\psi)$ could, in turn, be determined by the solution of its modelled transport equation but the computational effort involved would be out of all proportion to the information sought, namely $\tilde{\boldsymbol{\phi}}$. Consequently, a simpler method of determining $\tilde{p}(\psi)$ is required. Such a method would be to assume the shape of $\tilde{p}(\psi)$ based on the value of a finite number of its moments. This idea is not new. A variety of shapes have been suggested for the p.d.f. of a single passive scalar: a Gaussian (Hawthorne, Weddell & Hottel 1949), a beta function distribution (Richardson, Howard & Smith 1953, Rhodes 1975), a 'clipped Gaussian' (Lockwood & Naguib 1975) and a double delta function distribution (Bush & Fendell 1974; Khalil, Spalding & Whitelaw 1975). In the model of Bray & Moss (1974) a p.d.f. for a single reactive scalar is prescribed; Donaldson & Varma (1976) implicitly assume the joint p.d.f. of reactive scalars to be comprised of delta functions. All these distributions are determined as functions of the first and second moments for which modelled transport equations are solved.

For this approach to be generally applicable a method of determining $\tilde{p}(\psi)$ is required that (i) is applicable to reactive scalars, (ii) is applicable to any number of scalars, (iii) is mathematically correct, and that (iv) has physical justification.

Mathematical correctness requires that a valid p.d.f. can be determined from any valid set of moments, and that this p.d.f. should transform correctly. The method presented here meets all these requirements and has the additional advantage that extra information – third and fourth moments, for example – can be incorporated.

With a knowledge of the first and second moments, the following is known about $\tilde{p}(\psi)$:

$$\int \tilde{p}(\psi)\,\mathrm{d}\psi = 1, \tag{12.1}$$

$$\int \tilde{p}(\psi)\,\psi_\alpha\,\mathrm{d}\psi = \tilde{\phi}_\alpha, \tag{12.2}$$

and

$$\int \tilde{p}(\psi)\,(\psi_\alpha-\tilde{\phi}_\alpha)\,(\psi_\beta-\tilde{\phi}_\beta)\,\mathrm{d}\psi = C_{\alpha\beta} = \widetilde{\phi''_\alpha\,\phi''_\beta}. \tag{12.3}$$

Integration is over the whole of the accessible region outside which $\tilde{p}(\psi)$ is zero. With σ scalars, since $C_{\alpha\beta}$ is symmetric, there are $\frac{1}{2}(\sigma+1)\,(\sigma+2)$ of these integrals. Clearly there are many different p.d.fs that satisfy these $\frac{1}{2}(\sigma+1)\,(\sigma+2)$ constraints. How, then, is one distribution to be singled out? The only non-arbitrary assumption appears to be that $\tilde{p}(\psi)$ is the statistically most likely distribution subject to these constraints.

The details of the determination of the statistically most likely distribution are given by Pope (1979*b*). The entropy H of a distribution is defined by

$$H = -\int \tilde{p}(\psi)\ln[\tilde{p}(\psi)/q(\psi)]\,\mathrm{d}\psi \tag{12.4}$$

where $q(\psi)$ is the *a priori* probability. $q(\psi)$ is a positive quantity which represents the bias in composition space; if $q(\psi)$ is large, ϕ is biased towards that value of ψ, if $q(\psi)$ is small then ϕ is biased away from ψ. For passive scalars, it will be shown, there is no bias and so $q(\psi)$ is uniform. The specific form of $q(\psi)$ for reactive scalars is given below. H is introduced because a combinatorial analysis shows that the statistically most likely distribution is the one with the maximum entropy. An alternative view is that the distribution which maximises H contains a minimum of information. Any other distribution contains more information, therefore, and the additional information is spurious. Thus, it is assumed that $\tilde{p}(\psi)$ is the distribution that maximises H subject to the constraints, since this is the most likely distribution and the one that contains no spurious information.

The maximum entropy distribution subject to the constraints imposed by equations (12.1)–(12.3) is

$$\tilde{p}(\psi) = q(\psi)\exp\,(A_0+A_\alpha\psi_\alpha+B_{\alpha\beta}\psi_\alpha\psi_\beta). \tag{12.5}$$

The number of parameters (A and B) that have been introduced is $\frac{1}{2}(\sigma+1)\,(\sigma+2)$, the same as the number of constraints. Consequently A and B are determined by the values of $\tilde{\phi}_\alpha$ and $C_{\alpha\beta}$ and by the condition that $\tilde{p}(\psi)$ integrates to unity.

In one important case A and B can be determined explicitly. If the scalars are unbounded (the accessible region is infinite) and they are non-reactive ($q(\psi)$ = constant) the maximum entropy distribution is,

$$\tilde{p}(\psi) = (2\pi)^{-\frac{1}{2}\sigma}|C|^{-\frac{1}{2}}\exp\{-\tfrac{1}{2}C^{-1}_{\alpha\beta}(\psi_\alpha-\tilde{\phi}_\alpha)\,(\psi_\beta-\tilde{\phi}_\beta)\}. \tag{12.6}$$

This may be recognized as a σ-dimension Gaussian distribution.

For a single, bounded, non-reactive scalar the maximum entropy distribution is readily obtained by solving equations (12.1)–(12.3) and (12.5) by numerical means. Figures 5*a–c* show the resulting p.d.fs of temperature at three different radial locations in a heated axisymmetric jet. The maximum entropy distribution is shown as a full line and the points are taken from the experimental data of H. A. Moneib (1977, personal communication). Figure 5*a* corresponds to the edge of the jet, figure 5*c* to the centre-line, and figure 5*b* to a location in between. It may be seen that at the edge of the jet the p.d.f. is concentrated close to the lower bound where there is a spike. On the other hand, on the centre-line the distribution is little affected by either bound and, consequently, the maximum entropy distribution is nearly Gaussian. For both these positions, there is good quantitative agreement between the measurements and the predicted distribution. At the intermediate location, the distribution is clearly affected by the lower bound but there is no spike. In this instance, the discrepancy between the measurements and the maximum entropy distribution is more evident: but, considering that the distribution is based on only two moments, the agreement at all three locations is as good as can be expected.

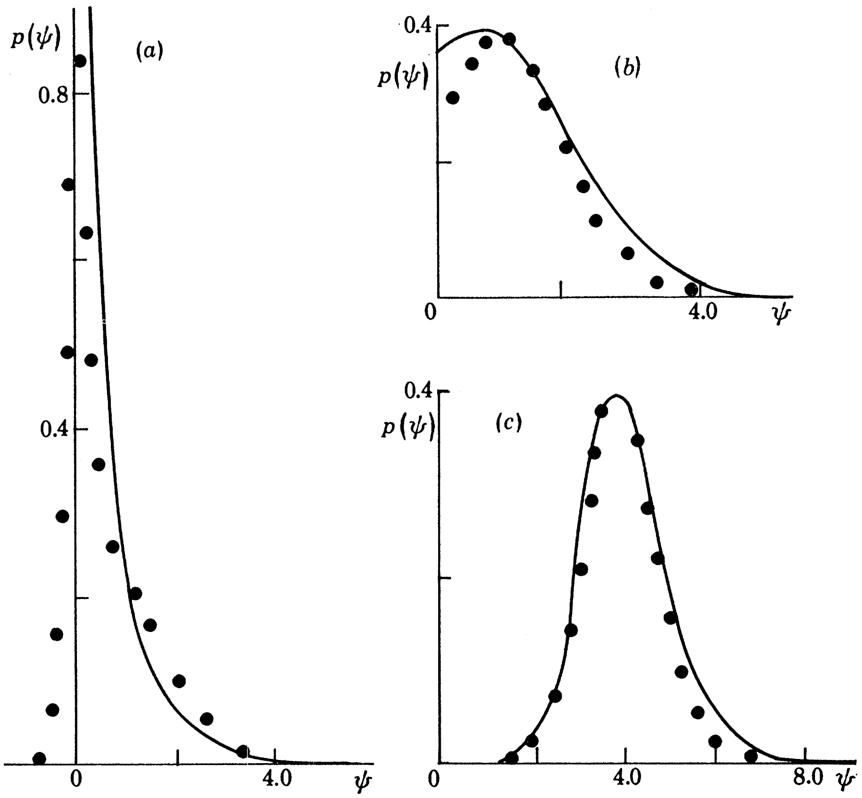

FIGURE 5. Graphs of $p(\psi)$ against ψ in an axisymmetric heated jet at $x/D = 22.0$; $\psi = (T-T_{\infty})/T'$. (*a*) $r/D = 3.6$; (*b*) $r/D = 2.6$; (*c*) $r/D = 0$.

For reactive scalars the *a priori* probability $q(\psi)$ is not uniform. In order to determine $q(\psi)$ we proceed in three stages: the general functional form of $q(\psi)$ is given; then, by considering the behaviour of $q(\psi)$ under linear transformations, the general functional form can be reduced to a functional of two invariants of ψ-space; and, finally, physical arguments are used to determine the specific form of this functional.

The only functions of composition space that appear in the conservation equations are the reaction rates and the density. It is to be expected therefore that $q(\psi)$ is a function of these quantities only. However, in order to confirm this expectation, it is supposed that $q(\psi)$ may be an intrinsic function of ψ as well: such an explicit dependence upon ψ will be shown to be inadmissible. In addition to ψ, $S_{\alpha}(\psi)$ and $\rho(\psi)$, a turbulent time scale τ, the correlation $C_{\alpha\beta}$ and the density $\langle\rho\rangle$ – none of which is a function of ψ – are used for normalization. Thus, $q(\psi)$ can be written as an unknown functional, Q',

$$q(\psi) = Q'(\psi, S_\alpha(\psi), \rho(\psi), \tau, C_{\alpha\beta}, \langle\rho\rangle). \tag{12.7}$$

$q(\psi)$ obeys the same transformation laws as $\tilde{p}(\psi)$, see § 10. With an asterisk denoting quantities in the linear transformed ψ^*-space,

$$|C|^{\frac{1}{2}} q(\psi) = |C^*|^{\frac{1}{2}} q^*(\psi^*), \tag{12.8}$$

and, since the functional form of q should be independent of the transformation,

$$|C|^{\frac{1}{2}} Q'(\psi, S_\alpha(\psi), \rho(\psi), \tau, C_{\alpha\beta}, \langle\rho\rangle) = |C^*|^{\frac{1}{2}} Q'(\psi^*, S^*_\alpha(\psi^*), \rho(\psi^*), \tau, C^*_{\alpha\beta}, \langle\rho\rangle). \tag{12.9}$$

Consequently, (12.7) can be rewritten as

$$q(\psi) = |C|^{-\frac{1}{2}} Q(I_1, I_2, \ldots, I_n), \tag{12.10}$$

where Q is an unknown functional and $I_1, I_2, \ldots, I_n$ are all the non-dimensional, invariant functions that can be formed from the arguments of Q'. There are only two invariants, $\rho(\psi)/\langle\rho\rangle$ and $X(\psi)$, where

$$X(\psi) = \tau\Omega(\psi) \tag{12.11}$$

and

$$\Omega^2(\psi) = C^{-1}_{\alpha\beta} S_\alpha(\psi) S_\beta(\psi). \tag{12.12}$$

$\Omega(\psi)$, it may be recalled, is the normalized speed along a path. Thus, the functional form of $q(\psi)$ can be reduced to,

$$q(\psi) = |C|^{-\frac{1}{2}} Q(X(\psi), \rho(\psi)/\langle\rho\rangle). \tag{12.13}$$

In constant-density, inert flows this relation becomes,

$$q(\psi) = |C|^{-\frac{1}{2}} Q(0, 1), \tag{12.14}$$

indicating that, although Q has not been specified, the *a priori* probability is uniform: the right hand side of equation (12.14) contains no dependence upon ψ. (The most likely candidate, $C^{-1}_{\alpha\beta}\psi_\alpha\psi_\beta$, is invariant under rotation and stretching but not under translation.) The general form of $q(\psi)$, equation (12.13) has been deduced without introducing any assumptions. Physical arguments are needed to determine the specific form.

As with other statistical quantities, that $\tilde{p}(\psi)$ behaves the same in variable-density flows as $p(\psi)$ does in constant-density flows seems to be the best available hypothesis. This argument was first put by Bilger (1975), and the works of Kent & Bilger (1977) and Bilger (1977) provide supporting evidence. This hypothesis implies that $q(\psi)$ is not a function of $\rho(\psi)$ and thus,

$$q(\psi) = |C|^{-\frac{1}{2}} Q(X(\psi)). \tag{12.15}$$

The determination of $Q(X)$ is guided by the following reasoning. Consider a particle moving randomly through a given space. If the particle is not biased towards any particular region of the space and if the behaviour of the particle is the same in all regions, then the probability of finding the particle in a given region is the same for all equally sized regions. In other words, if there is no bias then the *a priori* probability is uniform. Suppose, now, that there is some bias. Suppose, all other things being equal, that on average the particle travels through one region faster than through another. Since the time spent in a region is inversely proportional to the speed of travel through that region, the probability of finding a particle in the region is inversely proportional to its average speed. Thus, we conclude that the *a priori* probability at a point is inversely proportional to the average speed of transport at that point.

In composition space, transport is due to reaction and mixing. For a single scalar, a speed can readily be associated with each of these processes. With ϕ' as the standard deviation,

$$\phi' \equiv \widetilde{(\phi''\phi'')}^{\frac{1}{2}}, \tag{12.16}$$

the effect of mixing alone is to cause ϕ' to decay according to

$$\frac{\partial \phi'}{\partial t} = -\tfrac{1}{2}\epsilon_{\phi}/\phi' = -\phi'/\tau, \tag{12.17}$$

where this equation is used to define the turbulent time scale τ. According to the modelling of §7 (equation (7.16)), τ is

$$\tau = 2k/(C_{\phi 2}\epsilon). \tag{12.18}$$

Thus, ϕ'/τ is the speed of transport due to mixing. The speed due to reaction has already been identified as the speed along a path. In the case of a single scalar this is, simply, the absolute value of the reaction rate, $|S(\psi)|$.

Implementation of the principle that the *a priori* probability is inversely proportional to the speed leads to an expression for $q(\psi)$:

$$q(\psi) = \frac{1}{\phi'}\frac{\phi'/\tau}{(\phi'/\tau)+|S(\psi)|}. \tag{12.19}$$

Here, $(\phi'/\tau)+|S(\psi)|$ is the sum of the speeds and ϕ'/τ (in the numerator) is used for normalization. Or, dividing the numerator and denominator by ϕ'/τ, $q(\psi)$ can be rewritten as

$$q(\psi) = (1/\phi')\,(1+\tau|S(\psi)|/\phi')^{-1} \tag{12.20}$$

and then $\tau|S(\psi)|/\phi'$ is the ratio of the speeds.

This expression for $q(\psi)$ has been obtained from physical arguments. Is it, one may ask, consistent with the form of $q(\psi)$ deduced from the transformation properties (equation (12.15)), and can it be extended to more than one scalar? Both questions can be answered in the affirmative since the ratio of speeds is nothing but the invariant $X(\psi)$. Thus, the general expression for $q(\psi)$ is

$$q(\psi) = |C|^{-\frac{1}{2}}/(1+X(\psi)), \tag{12.21}$$

and $X(\psi)$ can be interpreted as the Euclidean norm of the ratio of the speeds. In a transform space in which $C_{\alpha\beta}$ is diagonal, $X(\psi)$ becomes,

$$X(\psi) = \tau\Big(\sum_{\alpha} S_{\alpha}(\psi)\, S_{\alpha}(\psi)/\widetilde{\phi''_{\alpha}\phi''_{\alpha}}\Big)^{\frac{1}{2}}. \tag{12.22}$$

The main points of this section are now summarized prior to a discussion. The statistically most likely distribution is that which maximises entropy (defined by equation (12.4)) subject to whatever constraints are imposed by the available information: equations (12.1)–(12.3) for example. The *a priori* probability $q(\psi)$, which appears in the definition of entropy, is uniform for non-reactive scalars. These are assumption free results. For reactive scalars, the properties of transformations in composition space lead to the functional form of $q(\psi)$ given by equation (12.13). Physical arguments suggest that $q(\psi)$ is not a function of $\rho(\psi)/\langle\rho\rangle$ and that its dependence upon $X(\psi)$ is given by equation (12.21).

The four requirements of a general method of determining an assumed distribution have been met. The method is applicable to any number of reactive or non-reactive scalars and it produces mathematically correct distributions. Its physical justification rests on the assumption that $\tilde{p}(\psi)$ is the statistically most likely distribution. Since any other assumption introduces extra (and therefore spurious) information, it appears that this is the best possible assumption. It is possible to imagine pathological cases in which the maximum entropy distribution (based on the first two moments) is far from the true distribution. This does not cast doubt on the assumption but rather indicates that in that case more information is required – third and fourth moments, for example. Such information could be incorporated as additional constraints on the maximization of entropy, and would result in cubic and quartic terms in the exponential of equation (12.5).

The validity of the expression for $q(\psi)$, equation (12.21), could be tested by comparing the resulting maximum entropy distribution either with measurements of $\tilde{p}(\psi)$ of with the solution of the modelled joint p.d.f. equation. Accurate measurements of $\tilde{p}(\psi)$ for reactive scalars are unlikely to be made for some time. Although there are still uncertainties in the modelled joint p.d.f. equation, the solutions can be expected to be quantitatively correct. Consequently a qualitative check on $q(\psi)$ could be obtained by solving the modelled equation for a simple case such as a homogeneous reaction. Since a quantitative check is not available, it is fortunate that the expression for $q(\psi)$ contains no undetermined function or constant.

D. Conclusion

13. *Summary*

The aim of this work has been to present and develop a theory which can be used to determine mean properties of turbulent flames. Attention has been focussed on the basic processes in relatively simple flames. Specifically, it is assumed that the Mach number is low and that the Reynolds number is high. Subject to these assumptions the properties at any point in the flame can be characterised by the velocity $\boldsymbol{U}(\boldsymbol{x}, t)$ and the set of scalars $\boldsymbol{\phi}(\boldsymbol{x}, t)$: these quantities are governed by equations (2.13)–(2.15). However, the solution of these equations with initial conditions and boundary conditions appropriate to turbulent flames is prohibitively difficult. Statistical theories attempt to describe the behaviour of averaged quantities in terms of averaged quantities. This requires the introduction of closure approximations, but renders a more readily solvable set of equations. It has been argued that a closure of the Reynolds-stress equations and the probability density function equation represents an optimum level of closure from the standpoint of physical insight. The conception of turbulent combustion that stems from the probability equations is one of transport in composition space: the consumption of a species by reaction corresponds to the transport of the p.d.f. to regions in composition space with lower values of that species. The use of the p.d.f. equation removes the difficulties that are otherwise encountered due to nonlinear functions of the scalars such as reaction rates. The computational expense of solving the modelled p.d.f. equation can be avoided by estimating the shape of the p.d.f. from its first and second moments. A general method has been presented for determining the statistically most likely distribution of any number of reactive or non-reactive scalars.

In order to close the Reynolds-stress equations three terms must be modelled: the pressure-rate of strain, the turbulent transport and the dissipation. The pressure-rate of strain term can be decomposed into two portions: the first, which is non-zero even in the absence of mean velocity gradients, has been modelled in most detail by Lumley & Newman (1977). Several models for the second part have been proposed, in the form of the mean velocity gradients multiplied by a function of the Reynolds stresses. Of these, the proposal of Launder, Reece & Rodi (1975) is probably the most general model that can be justified with the present experimental data. Turbulent transport of Reynolds stress is caused by gradients of the triple velocity correlations and also by pressure velocity correlation gradients. It has been suggested that, until uncertainties in other areas of the model are reduced, simple gradient diffusion may provide an adequate description of the transport.

Dissipation is determined from its own transport equation. ϵ can be regarded as the rate of transfer of energy from the energy-containing motions, and is governed by inertia, not by molecular processes. The source in the dissipation equation given by Lumley (1975*a*) appears to account for similar flows with and without shear. The additional term proposed by Pope (1978) overcomes the previously encountered discrepancy for the round jet.

In the transport equations for the first and second moments of ϕ, the scalar flux $\langle u_i \phi'_\alpha \rangle$ is the dominant unknown. Its gradient accounts for the transport of $\langle \phi_\alpha \rangle$ and multiplied by the mean scalar gradient it represents the production of $\langle \phi'_\alpha \phi'_\beta \rangle$. The transport equation for the scalar flux is similar to that for the Reynolds stresses and similar modelling has been proposed. There is some uncertainty in modelling the dissipation of scalar fluctuations $\epsilon_{\alpha\beta}$: the data indicate that the contention that $\epsilon_{\alpha\beta}$ is proportional to ϵ and $\langle \phi'_\alpha \phi'_\beta \rangle$ can be in error by 50%. Consequently, proposals have been made for a modelled transport equation for $\epsilon_{\alpha\beta}$. This is sound in principle, but because of modelling uncertainties there is no reason to believe that this will produce more accurate results.

The behaviour of statistical equations in variable-density flows may differ from that of their constant-density counterparts because of the appearance of additional terms, and because existing terms behave differently. The use of density-weighted averaging generally ensures that no additional terms arise. Also, since their transport equations retain conservative form, density-weighted quantities may be expected to behave similarly in constant-density and variable-density flows. There is no shortage of suggested additions to models to account for density variations. The shortage is of definitive experimental data by which such additions can be tested. At present, there is no strong case for believing that any additional term would enhance the accuracy of any modelled equation. In comparing measured and calculated values in variable-density flows, it is essential to compare like with like. It is relatively easy to convert from density-weighted to unweighted quantities (or vice versa) in a calculation, but less so in experiments. Means of conversion are given in §8.

Second order closures can be expected to be accurate for near-equilibrium, nearly-homogeneous flows. Although this assessment is imprecise, this level of closure can be expected to be adequate for free shear flows. A considerable amount of work needs to be done in order to produce a more accurate and general second order turbulence closure. Such work is being performed in several centres and those involved are not in need of suggestions: what is required is the painstaking evaluation and development of existing proposals. The only area that seems to be receiving less attention than it deserves is that of variable-density flows. Although relevant experimental data are far from abundant, there are sufficient to provide useful tests of the models

The joint p.d.f. $p(\psi)$ is a distribution in ψ-space, the composition space. A value of ψ corresponds to a gas mixture of composition $\phi(x, t) = \psi$. ψ-space is bounded since only some compositions are allowed. For example, negative mass fractions clearly are disallowed. In a particular flame not all the allowed compositions may be accessible. The accessible region, outside which $p(\psi)$ is zero, is defined in §10. Chemical reaction in a homogeneous (non-turbulent) mixture proceeds along reaction paths in composition space.

The transport equation for the density-weighted joint p.d.f. indicates that $\tilde{p}(\psi)$ is convected in position space by the mean flow and by turbulence and is transported in composition space by reaction and by molecular mixing. A consistent model for the turbulent flux $\widetilde{p'(\psi)u_i''}$ has been proposed. The effect of reaction (which appears in closed form) is to transport probability along reaction paths in composition space. In the absence of other effects, molecular action causes the second moments of $\tilde{p}(\psi)$ to decrease without changing the mean values $\tilde{\phi}_\alpha$. In the limit as $\tilde{p}(\psi)$ tends to a delta function it is presumed to do so as a Gaussian and consequently all cumulants tend to zero. Models which produce the correct qualitative performance take the form of integrals over the composition space and are, therefore, computationally expensive. None of these models has been shown to produce the correct Gaussian asymptote.

Rather than solving the computationally-expensive modelled transport equation for $\tilde{p}(\psi)$ it has been suggested that $\tilde{p}(\psi)$ can be estimated from a finite number of its moments. A general method has been presented for determining the statistically most likely distribution. This is achieved by maximising entropy subject to the constraints imposed by the first and second moments. The *a priori* probability $q(\psi)$, which appears in the definition of entropy, is uniform for passive scalars. For reactive scalars, $q(\psi)$ is a function of the two invariants of composition space, and physical arguments have been used to determine the specific form of this function.

APPENDIX. THE DERIVATION OF DENSITY-WEIGHTED EQUATIONS

A general method of deriving density-weighted equations is presented. It results in the general equations (A 6) and (A 20) which are used to obtain the equations given in the text.

A general quantity expressed as a function of the dependent variables, $Q(U, \phi)$, is considered first. Then functions of fluctuating components of the dependent variables, $R(\mathbf{u}'', \phi'')$, are treated. Within the first class are the mean quantities themselves, $\tilde{U}_j$ and $\tilde{\phi}_\alpha$, and within the second are the velocity and scalar correlations $\widetilde{u_i''u_j''}$, $\widetilde{u_i''\phi_\alpha''}$ and $\widetilde{\phi_\alpha''\phi_\beta''}$. Finally, the transport equation for the joint probability density function of the scalars $\tilde{p}(\psi)$ is derived.

Functions of $\tilde{\boldsymbol{U}}$ and $\tilde{\boldsymbol{\phi}}$

Defining,

$$\frac{\mathrm{D}}{\mathrm{D}t} \equiv \frac{\partial}{\partial t} + U_i \frac{\partial}{\partial x_i}, \tag{A 1}$$

and

$$\frac{\tilde{\mathrm{D}}}{\mathrm{D}t} \equiv \frac{\partial}{\partial t} + \tilde{U}_i \frac{\partial}{\partial x_i}, \tag{A 2}$$

then, for any quantity Q,

$$\left\langle \rho \frac{\mathrm{D}Q}{\mathrm{D}t} \right\rangle = \left\langle \frac{\partial \rho Q}{\partial t} + \frac{\partial \rho U_i Q}{\partial x_i} \right\rangle = \frac{\partial \langle \rho \rangle \tilde{Q}}{\partial t} + \frac{\partial (\langle \rho \rangle \tilde{U}_i \tilde{Q} + \langle \rho \rangle \widetilde{u_i'' Q})}{\partial x_i} = \langle \rho \rangle \frac{\tilde{\mathrm{D}} \tilde{Q}}{\mathrm{D}t} + \frac{\partial \langle \rho \rangle \widetilde{u_i'' Q}}{\partial x_i}. \tag{A 3}$$

In (A 3) use has been made of the instantaneous continuity equations (2.1) and its mean,

$$\frac{\partial \langle \rho \rangle}{\partial t} + \frac{\partial \langle \rho \rangle \tilde{U}_i}{\partial x_i} = 0. \tag{A 4}$$

For any function of $\boldsymbol{U}$ and $\boldsymbol{\phi}$, $Q(\boldsymbol{U}, \boldsymbol{\phi})$, the left hand side of (A 3) may be rewritten

$$\left\langle \rho \frac{\mathrm{D}Q(\boldsymbol{U}, \boldsymbol{\phi})}{\mathrm{D}t} \right\rangle = \left\langle \frac{\partial Q(\boldsymbol{U}, \boldsymbol{\phi})}{\partial U_i} \rho \frac{\mathrm{D}U_i}{\mathrm{D}t} \right\rangle + \left\langle \frac{\partial Q(\boldsymbol{U}, \boldsymbol{\phi})}{\partial \phi_\alpha} \rho \frac{\mathrm{D}\phi_\alpha}{\mathrm{D}t} \right\rangle, \tag{A 5}$$

where summation is over all α. Thus, combining (A 3) and (A 5) gives the density-weighted transport equation for $Q(\boldsymbol{U}, \boldsymbol{\phi})$:

$$\langle\rho\rangle\frac{\widetilde{\mathrm{D}}\widetilde{Q}}{\mathrm{D}t}+\frac{\partial\langle\rho\rangle\widetilde{u_i''Q}}{\partial x_i}=\left\langle\frac{\partial Q}{\partial U_i}\rho\frac{\mathrm{D}U_i}{\mathrm{D}t}\right\rangle+\left\langle\frac{\partial Q}{\partial\phi_\alpha}\rho\frac{\mathrm{D}\phi_\alpha}{\mathrm{D}t}\right\rangle. \tag{A 6}$$

The mean velocity equation

With

$$Q(\boldsymbol{U},\boldsymbol{\phi})\equiv U_j, \tag{A 7}$$

then

$$\widetilde{Q}(\boldsymbol{U},\boldsymbol{\phi})=\widetilde{U}_j, \tag{A 8}$$

$$\widetilde{u_i''Q(\boldsymbol{U},\boldsymbol{\phi})}=\widetilde{u_i''U_j}=\widetilde{u_i''u_j''}, \tag{A 9}$$

$$\frac{\partial Q(\boldsymbol{U},\boldsymbol{\phi})}{\partial U_i}=\delta_{ij}, \tag{A 10}$$

and

$$\frac{\partial Q(\boldsymbol{U},\boldsymbol{\phi})}{\partial\phi_\alpha}=0. \tag{A 11}$$

Substitution of equations (A 8)–(A 11) into equation (A 6) yields

$$\langle\rho\rangle\frac{\widetilde{\mathrm{D}}\widetilde{U}_j}{\mathrm{D}t}+\frac{\partial\langle\rho\rangle\widetilde{u_i''u_j''}}{\partial x_i}=\left\langle\rho\frac{\mathrm{D}U_j}{\mathrm{D}t}\right\rangle. \tag{A 12}$$

Replacing $\rho\mathrm{D}U_j/\mathrm{D}t$ by the right hand side of equation (2.13) gives the mean velocity equation

$$\langle\rho\rangle\frac{\widetilde{\mathrm{D}}\widetilde{U}_j}{\mathrm{D}t}+\frac{\partial\langle\rho\rangle\widetilde{u_j''u_i''}}{\partial x_i}=\frac{\partial}{\partial x_i}\mu\left(\frac{\partial\langle U_i\rangle}{\partial x_j}+\frac{\partial\langle U_j\rangle}{\partial x_i}\right)-\frac{\partial\langle p\rangle}{\partial x_j}+\langle\rho\rangle g_j. \tag{A 13}$$

The mean scalar equation

With

$$Q(\boldsymbol{U},\boldsymbol{\phi})\equiv\phi_\alpha \tag{A 14}$$

a similar procedure yields

$$\langle\rho\rangle\frac{\widetilde{\mathrm{D}}\widetilde{\phi}_\alpha}{\mathrm{D}t}+\frac{\partial\langle\rho\rangle\widetilde{u_i''\phi_\alpha''}}{\partial x_i}=\left\langle\rho\frac{\mathrm{D}\phi_\alpha}{\mathrm{D}t}\right\rangle \tag{A 15}$$

and, from equation (2.14) the mean scalar equation is

$$\langle\rho\rangle\frac{\widetilde{\mathrm{D}}\widetilde{\phi}_\alpha}{\mathrm{D}t}+\frac{\partial\langle\rho\rangle\widetilde{u_i''\phi_\alpha''}}{\partial x_i}=\frac{\partial}{\partial x_i}\Gamma\frac{\partial\langle\phi_\alpha\rangle}{\partial x_i}+\langle\rho\rangle\widetilde{S}_\alpha(\boldsymbol{\phi}). \tag{A 16}$$

For these two cases, the method is almost trivial but its advantages are evident for more involved functions.

Functions of $\boldsymbol{U}''$ and ϕ''

For any function of $\boldsymbol{u}''$ and $\boldsymbol{\phi}''$, $R(\boldsymbol{u}'', \boldsymbol{\phi}'')$, the form of equation ($A$ 3) holds; that is

$$\left\langle\rho\frac{\mathrm{D}R}{\mathrm{D}t}\right\rangle=\langle\rho\rangle\frac{\widetilde{\mathrm{D}}\widetilde{R}}{\mathrm{D}t}+\frac{\partial}{\partial x_i}\langle\rho\rangle\widetilde{u_i''R}. \tag{A 17}$$

Expanding the left hand side gives

$$\left\langle\rho\frac{\mathrm{D}R}{\mathrm{D}t}\right\rangle=\left\langle\rho\frac{\partial R}{\partial u_i''}\frac{\mathrm{D}u_i''}{\mathrm{D}t}\right\rangle+\left\langle\rho\frac{\partial R}{\partial\phi_\alpha''}\frac{\mathrm{D}\phi_\alpha''}{\mathrm{D}t}\right\rangle. \tag{A 18}$$

Now,

$$\frac{\mathrm{D}\phi_\alpha''}{\mathrm{D}t}=\frac{\mathrm{D}\phi_\alpha}{\mathrm{D}t}-\frac{\mathrm{D}\widetilde{\phi}_\alpha}{\mathrm{D}t}=\frac{\mathrm{D}\phi_\alpha}{\mathrm{D}t}-\frac{\widetilde{\mathrm{D}}\widetilde{\phi}_\alpha}{\mathrm{D}t}-u_j''\frac{\partial\widetilde{\phi}_\alpha}{\partial x_j}. \tag{A 19}$$

Thus, combining equations (*A* 17) and (*A* 18), with $\mathrm{D}\phi''_\alpha/\mathrm{D}t$ given by (*A* 19), and similarly for $\mathrm{D}u''_i/\mathrm{D}t$, produces the transport equation for R:

$$\langle\rho\rangle\frac{\tilde{\mathrm{D}}\tilde{R}}{\mathrm{D}t}+\frac{\partial\langle\rho\rangle\widetilde{u''_i R}}{\partial x_i}+\langle\rho\rangle\frac{\partial\tilde{U}_l}{\partial x_i}\widetilde{u''_i\frac{\partial R}{\partial u''_l}}+\langle\rho\rangle\frac{\partial\tilde{\phi}_\alpha}{\partial x_i}\widetilde{u''_i\frac{\partial R}{\partial\phi''_\alpha}}$$
$$=\left\langle\frac{\partial R}{\partial u''_i}\rho\frac{\mathrm{D}U_i}{\mathrm{D}t}\right\rangle-\widetilde{\frac{\partial R}{\partial u''_i}}\langle\rho\rangle\frac{\tilde{\mathrm{D}}\tilde{U}_i}{\mathrm{D}t}+\left\langle\frac{\partial R}{\partial\phi''_\alpha}\rho\frac{\mathrm{D}\phi_\alpha}{\mathrm{D}t}\right\rangle-\widetilde{\frac{\partial R}{\partial\phi''_\alpha}}\langle\rho\rangle\frac{\tilde{\mathrm{D}}\tilde{\phi}_\alpha}{\mathrm{D}t}. \qquad (A\ 20)$$

The Reynolds-stress equation

With
$$R(\boldsymbol{u}'',\boldsymbol{\phi}'')=u''_j u''_k, \qquad (A\ 21)$$
then
$$\tilde{R}=\widetilde{u''_j u''_k}, \qquad (A\ 22)$$
$$\widetilde{Ru''_i}=\widetilde{u''_i u''_j u''_k}, \qquad (A\ 23)$$
$$\widetilde{u''_i\frac{\partial R}{\partial u''_l}}=\widetilde{u''_i u''_j}\,\delta_{lk}+\widetilde{u''_i u''_k}\,\delta_{lj}, \qquad (A\ 24)$$
$$\frac{\partial R}{\partial u''_l}=u''_j\,\delta_{lk}+u''_k\,\delta_{lj}, \qquad (A\ 25)$$
$$\widetilde{\frac{\partial R}{\partial u''_l}}=0, \qquad (A\ 26)$$
and
$$\frac{\partial R}{\partial\phi''_\alpha}=0. \qquad (A\ 27)$$

Substituting these relations into equation (*A* 20) gives

$$\langle\rho\rangle\frac{\tilde{\mathrm{D}}\widetilde{u''_j u''_k}}{\mathrm{D}t}+\frac{\partial\langle\rho\rangle\widetilde{u''_i u''_j u''_k}}{\partial x_i}+\langle\rho\rangle\widetilde{u''_i u''_j}\frac{\partial\tilde{U}_k}{\partial x_i}+\langle\rho\rangle\widetilde{u''_i u''_k}\frac{\partial\tilde{U}_j}{\partial x_i}$$
$$=-\left\langle u''_j\rho\frac{\mathrm{D}U_k}{\mathrm{D}t}\right\rangle+\left\langle u''_k\rho\frac{\mathrm{D}U_j}{\mathrm{D}t}\right\rangle$$
$$=-\left\langle u''_j\frac{\partial p}{\partial x_k}\right\rangle-\left\langle u''_k\frac{\partial p}{\partial x_j}\right\rangle+\left\langle u''_j\frac{\partial}{\partial x_i}\mu\left(\frac{\partial U_k}{\partial x_i}+\frac{\partial U_i}{\partial x_k}\right)\right\rangle+\left\langle u''_k\frac{\partial}{\partial x_i}\mu\left(\frac{\partial U_j}{\partial x_i}+\frac{\partial U_i}{\partial x_j}\right)\right\rangle. \qquad (A\ 28)$$

where $\mathrm{D}U_k/\mathrm{D}t$ has been taken from equation (2.13).

The scalar correlation equation

The density-weighted equation for $\widetilde{\phi''_\alpha\phi''_\beta}$ is obtained in a directly analogous way with the substitution
$$R(\boldsymbol{u}'',\boldsymbol{\phi}'')\equiv\phi''_\alpha\phi''_\beta. \qquad (A\ 29)$$
The result is

$$\langle\rho\rangle\frac{\tilde{\mathrm{D}}\widetilde{\phi''_\alpha\phi''_\beta}}{\mathrm{D}t}+\frac{\partial\langle\rho\rangle\widetilde{u''_i\phi''_\alpha\phi''_\beta}}{\partial x_i}+\langle\rho\rangle\widetilde{u''_i\phi''_\alpha}\frac{\partial\tilde{\phi}_\beta}{\partial x_i}+\langle\rho\rangle\widetilde{u''_i\phi''_\beta}\frac{\partial\tilde{\phi}_\alpha}{\partial x_i}$$
$$=\left\langle\phi''_\alpha\rho\frac{\mathrm{D}\phi_\beta}{\mathrm{D}t}\right\rangle+\left\langle\phi''_\beta\rho\frac{\mathrm{D}\phi_\alpha}{\mathrm{D}t}\right\rangle$$
$$=\langle\rho\rangle\widetilde{\phi''_\alpha S_\beta(\boldsymbol{\phi})}+\langle\rho\rangle\widetilde{\phi''_\beta S_\alpha(\boldsymbol{\phi})}+\left\langle\phi''_\alpha\frac{\partial}{\partial x_i}\Gamma\frac{\partial\phi_\beta}{\partial x_i}\right\rangle+\left\langle\phi''_\beta\frac{\partial}{\partial x_i}\Gamma\frac{\partial\phi_\alpha}{\partial x_i}\right\rangle. \qquad (A\ 30)$$

The scalar-flux equation

The transport equation for the scalar-flux, $\widetilde{u_j'' \phi_\alpha''}$ is obtained by the substitution of

$$R(\boldsymbol{u}'', \boldsymbol{\phi}'') = u_j'' \phi_\alpha'' \tag{A 31}$$

into equation (A 20):

$$\begin{aligned}\langle\rho\rangle \frac{\widetilde{\mathrm{D}}\widetilde{u_j''\phi_\alpha''}}{\mathrm{D}t} + \frac{\partial\langle\rho\rangle \widetilde{u_i''u_j''\phi_\alpha''}}{\partial x_i} + \langle\rho\rangle \widetilde{u_i''\phi_\alpha''}\frac{\partial \tilde{U}_j}{\partial x_i} + \langle\rho\rangle \widetilde{u_i''u_j''}\frac{\partial\tilde{\phi}_\alpha}{\partial x_i} \\ = \left\langle u_j'' \rho \frac{\mathrm{D}\phi_\alpha}{\mathrm{D}t}\right\rangle + \left\langle \phi_\alpha'' \rho \frac{\mathrm{D}U_j}{\mathrm{D}t}\right\rangle \\ = -\left\langle \phi_\alpha'' \frac{\partial p}{\partial x_j}\right\rangle + \langle\rho\rangle \widetilde{u_j'' S_\alpha(\boldsymbol{\phi})} + \left\langle \phi_\alpha'' \frac{\partial}{\partial x_i}\mu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)\right\rangle + \left\langle u_j'' \frac{\partial}{\partial x_i}\Gamma\frac{\partial\phi_\alpha}{\partial x_j}\right\rangle.\end{aligned} \tag{A 32}$$

The probability density function equation

The joint probability distribution of σ scalars ϕ_α ($\alpha = 1, \sigma$) is given by

$$p(\psi; \boldsymbol{x}, t) \equiv \langle \delta(\psi - \boldsymbol{\phi}(\boldsymbol{x}, t))\rangle \tag{A 33}$$

where

$$\delta(\psi - \boldsymbol{\phi}(\boldsymbol{x}, t)) \equiv \prod_{\alpha=1}^{\sigma} \delta(\psi_\alpha - \phi_\alpha(\boldsymbol{x}, t)), \tag{A 34}$$

δ being the Dirac delta function. Thus, from (A 3),

$$\left\langle \rho \frac{\mathrm{D}\delta(\psi - \boldsymbol{\phi})}{\mathrm{D}t}\right\rangle = \langle\rho\rangle \frac{\widetilde{\mathrm{D}}\tilde{p}(\psi)}{\mathrm{D}t} + \frac{\partial\langle\rho\rangle \widetilde{u_i''\delta(\psi - \boldsymbol{\phi})}}{\partial x_i}, \tag{A 35}$$

where $\tilde{p}(\psi)$ is the density-weighted p.d.f.

$$\langle\rho\rangle \tilde{p}(\psi) = \langle \rho(\boldsymbol{\phi})\, \delta(\psi - \boldsymbol{\phi})\rangle = \rho(\psi)\, p(\psi). \tag{A 36}$$

The left-hand side of (A 35) may be expanded as

$$\begin{aligned}\left\langle \rho \frac{\mathrm{D}\delta(\psi - \boldsymbol{\phi})}{\mathrm{D}t}\right\rangle = \left\langle \rho \frac{\partial\delta(\psi - \boldsymbol{\phi})}{\partial\phi_\alpha}\frac{\mathrm{D}\phi_\alpha}{\mathrm{D}t}\right\rangle = -\left\langle \rho \frac{\partial\delta(\psi - \boldsymbol{\phi})}{\partial\psi_\alpha}\frac{\mathrm{D}\phi_\alpha}{\mathrm{D}t}\right\rangle \\ = -\frac{\partial}{\partial\psi_\alpha}\left\langle \delta(\psi - \boldsymbol{\phi})\, \rho \frac{\mathrm{D}\phi_\alpha}{\mathrm{D}t}\right\rangle,\end{aligned} \tag{A 37}$$

which combined with (A 35) gives the transport equation for $\tilde{p}(\psi)$:

$$\begin{aligned}\langle\rho\rangle \frac{\widetilde{\mathrm{D}}\tilde{p}(\psi)}{\mathrm{D}t} + \frac{\partial\langle\rho\rangle \widetilde{u_i''\delta(\psi - \boldsymbol{\phi})}}{\partial x_i} = -\frac{\partial}{\partial\psi_\alpha}\left\langle \delta(\psi - \boldsymbol{\phi})\, \rho \frac{\mathrm{D}\phi_\alpha}{\mathrm{D}t}\right\rangle \\ = -\frac{\partial\langle\rho\rangle \tilde{p}(\psi)\, S_\alpha(\psi)}{\partial\psi_\alpha} - \frac{\partial}{\partial\psi_\alpha}\left\langle \delta(\psi - \boldsymbol{\phi})\frac{\partial}{\partial x_i}\Gamma\frac{\partial\phi_\alpha}{\partial x_i}\right\rangle.\end{aligned} \tag{A 38}$$

Or finally, writing $p'(\psi)$ for $\delta(\psi - \boldsymbol{\phi})$,

$$\langle\rho\rangle \frac{\widetilde{\mathrm{D}}\tilde{p}(\psi)}{\mathrm{D}t} + \frac{\partial\langle\rho\rangle \widetilde{u_i''p'(\psi)}}{\partial x_i} = -\frac{\partial\langle\rho\rangle \tilde{p}(\psi)\, S_\alpha(\psi)}{\partial\psi_\alpha} - \frac{\partial}{\partial\psi_\alpha}\left\langle p'(\psi)\frac{\partial}{\partial x_i}\Gamma\frac{\partial\phi_\alpha}{\partial x_i}\right\rangle. \tag{A 39}$$

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