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Second-order modelling of a variable-density mixing layer

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A conventional (non-density-weighted) averaging method is used to study variable-density turbulent flows, in particular, a helium–nitrogen mixing layer. A careful order-of-magnitude analysis is carried out, first in relative density fluctuations, and then in the ratio of cross-stream to streamwise lengthscales. In this way it is shown that, to lowest order, in jets and shear layers, the turbulence is unafffected by the density fluctuations, and conventional models can be used. The non-uniform density distribution influences only the mean-continuity and mean-momentum equations. Calculations (using a new form for the scalar-dissipation equation based on relaxation to an equilibrium timescale ratio) show good agreement with experiment. Calculation with a less truncated system indicates that neglected terms have little effect. We use a modified Patankar–Spalding method that overcomes numerical stability difficulties.

1. Introduction

Variable-density turbulent flows have been studied using various averaging schemes. To the second-order closure level, there are at least three schemes. The first is conventional averaging. Donaldson, Sullivan & Rosenbaum (1972), Janicka & Kollmann (1979), Janicka & Lumley (1981) use conventional averaging to study variable density flows with models that are developed in different ways. The second was originally proposed by Favre (1966, 1969) and is called density-weighted averaging or Favre averaging. Many authors (Kent & Bilger 1976; Borghi & Dutoya 1978; Jones 1979; Libby 1977; Vandromme 1980) use this method to study variable-density turbulent flow with models that are essentially developed in constant-density turbulent flow. The third is the so-called mixed-weighted averaging used by Ha Minh, Launder & MacInnes (1981).

Here we follow Janicka & Lumley's (1981) idea to study the variable-density turbulent mixing layer, in which there are strong density fluctuations. The experimental studies of Rebollo (1973) and Konrad (1976) will provide an assessment of this model scheme.

The full set of equations for the variable-density mixing layer will contain mean velocity, mean mass fraction, Reynolds stress, flux of mass-fraction fluctuation, turbulent energy, variance of mass-fraction fluctuation, dissipation of turbulent

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energy and dissipation of variance of mass-fraction fluctuation. First, we carry out an expansion in relative density fluctuation, keeping lowest-order terms, justifying this on the basis of observed values of the r.m.s. density fluctuation. For all but the pressure correlations, it is possible at this point to show that conventional models are, to first order, adequate. Using conventional pressure correlation models, these modelled equations provide our more complete set.

We then proceed to an order-of-magnitude analysis of jets and shear layers, beginning from our more complete model. We find that the conventional pressure correlation model is indeed appropriate to lowest order, and that in fact to this order the turbulence is in local equilibrium and is unaffected by the density fluctuations, which are produced passively from the mean gradient. The density non-uniformity influences only the mean-continuity and mean-momentum equations. The local equilibrium results in algebraic Reynolds-stress and flux equations. This is our simplified set. The solutions of the more complete and the very simple sets of modelled equations are quite close, and both are in reasonable agreement with experimental data. In the following sections we shall describe the basic equations, models, numerical methods and results.

2. Basic equations

We shall concentrate on variable-density flow in which the density fluctuations are caused only by mixing gases with different densities. In this case the density of the mixed gas is only a function of the mass fraction f, defined by

$$\rho = \frac{1}{cf+e}, \tag{2.1}$$

$$c = \frac{1}{\rho_1} - \frac{1}{\rho_2}, \quad e = \frac{1}{\rho_2},$$

where ρ is the density of mixed gas, and ρ_1 and ρ_2 are the densities of the two different gas species. Let us write the kinematic diffusivity of mixed gas as d. We may assume that this diffusivity is approximately independent of mass fraction f (see Jeans 1954). Now for isothermal flow the diffusivity d and viscosity μ will be considered as constants in the flow field. The general equations governing instantaneous quantities are as follows:

$$f_{,t} + u_k f_{,k} = \frac{1}{\rho}(d\rho f_{,k})_{,k}, \tag{2.2}$$

$$u_{i,t} + u_j u_{i,j} = -\frac{1}{\rho}[p + \tfrac{2}{3}\mu u_{p,p}]_{,i} + \nu(u_{i,j} + u_{j,i})_{,j} + g_i, \tag{2.3}$$

$$\rho_{,t} + (\rho u_k)_{,k} = 0. \tag{2.4}$$

Equation (2.2) is the conservation equation of mass fraction, (2.3) is the momentum equation and (2.4) is the continuity equation; g_i stands for the gravity vector.

For the conventional averaging method, we decompose all the instantaneous quantities into mean and fluctuating parts:

$$\rho = \langle\rho\rangle + \rho', \quad f = F + f', \quad u_i = U_i + u_i', \quad p = P + p'. \tag{2.5}$$

Before we derive the equations for the various statistical quantities, let us look at the relation between density fluctuations and mass-fraction fluctuations which we shall need in the following sections.

If we rewrite (2.1) as

$$cf+e=\frac{1}{\rho}$$
$$=\frac{1}{\langle\rho\rangle+\rho'}$$
$$=\frac{1}{\langle\rho\rangle}\left[1-\frac{\rho'}{\langle\rho\rangle}+\left(\frac{\rho'}{\langle\rho\rangle}\right)^2+\dots\right]$$

we obtain

$$cF+e=\frac{1}{\langle\rho\rangle}\left[1+\left\langle\left(\frac{\rho'}{\langle\rho\rangle}\right)^2\right\rangle-\dots\right],$$
$$cf'=\frac{1}{\langle\rho\rangle}\left[-\frac{\rho'}{\langle\rho\rangle}+\left(\frac{\rho'}{\langle\rho\rangle}\right)^2-\left\langle\left(\frac{\rho'}{\langle\rho\rangle}\right)^2\right\rangle+\dots\right],$$

where $\langle\ \rangle$ stands for averaging. To simplify the problem, we assume that ρ' is of order of its r.m.s. ρ'', and $\rho''/\langle\rho\rangle$ is small compared with 1. In fact, we shall see that $\rho''/\langle\rho\rangle$ in the He/N mixing layer never rises above 0.45 and reaches that value only in a narrow zone. In non-premixed flames (Chen & Lumley 1984) $\rho''/\langle\rho\rangle$ is found to be no larger than 0.4, again reaching this value only in a narrow zone. Levels of 0.4 for $\rho''/\langle\rho\rangle$ suggest maximum errors of 16% in relatively narrow regions, which is satisfactory for many purposes. It is fair to say that, generally speaking, relative density fluctuations of order 0.4 are rare, so that the model performance will generally be better than this. Certainly we can in this way arrive at an understanding of the physics. After neglecting higher-order terms in $\rho''/\langle\rho\rangle$ we obtain

$$\langle\rho\rangle=\frac{1}{cF+e}+O\left(\frac{\rho''}{\langle\rho\rangle}\right)^2, \tag{2.6}$$

$$\frac{\rho'}{\langle\rho\rangle}=-c\langle\rho\rangle f'+O\left(\frac{\rho''}{\langle\rho\rangle}\right)^2. \tag{2.7}$$

Equation (2.7) is a useful relation to form the correlation between density and other quantities. In the derivation of all mean and second-moment equations, we shall also use the following approximation: $1/\rho=(1/\langle\rho\rangle)(1-\rho'/\langle\rho\rangle)+O(\rho''/\langle\rho\rangle)^2$. In a variable-density flow the divergence of velocity is not zero. We may obtain its mean and fluctuating parts from (2.4), (2.1) and (2.2):

$$U_{k,k}=dc(\langle\rho\rangle F_{,k}+\langle\rho' f'_{,k}\rangle)_{,k},$$
$$u'_{k,k}=dc(\langle\rho\rangle f'_{,k}+\rho' F_{,k}+\rho' f'_{,k}-\langle\rho' f'_{,k}\rangle)_{,k}.$$

In order to simplify these expressions we apply two types of order-of-magnitude analysis. One is related to (2.7); i.e. $c\langle\rho\rangle f'$ ($\approx\rho'/\langle\rho\rangle$) is considered as a small quantity. The other is related to the assumption of high turbulent Reynolds number and Schmidt number, such that $\langle u'_{i,j}f'_{,j}\rangle/\langle u'_i f'_{,j}\rangle_{,j}\approx R_l^{\frac{1}{2}}$, where $R_l=u'l/\nu$, $3u'^2=\langle q^2\rangle$, $l=u'^3/\langle\epsilon\rangle$, and $\langle q^2\rangle$ and $\langle\epsilon\rangle$ are the turbulent kinetic energy and dissipation respectively. This kind of order-of-magnitude analysis will be applied in the derivation of various equations. Clearly if we only keep the terms of order $c\langle\rho\rangle f'$

and keep the assumption of high turbulent Reynolds/Schmidt number in mind during the averging process, then we shall obtain

$$U_{k,k} = dc(\langle\rho\rangle F_{,kk} - \langle\rho\rangle^2 F_{,k} F_{,k}), \tag{2.8}$$

$$u'_{k,k} = dc\langle\rho\rangle f'_{,kk}. \tag{2.9}$$

Now let us derive the equations for the following statistical quantities: mean velocity, mean mass fraction, Reynolds stress, flux of mass fraction, mass-fraction variance, dissipation of turbulent energy and dissipation of mass-fraction variance. Decomposing the quantities in (2.2), we have

$$\begin{aligned} F_{,t} + f'_{,t} + U_k F_{,k} + u'_k F_{,k} + U_k f'_{,k} + u'_k f'_{,k} \\ = dF_{,kk} + df'_{,kk} + \frac{d}{\langle\rho\rangle}(\langle\rho\rangle_{,k} F_{,k} + \rho'_{,k} f'_{,k} + \langle\rho\rangle_{,k} f'_{,k} + F_{,k}\rho'_{,k}) \\ + \frac{d}{\langle\rho\rangle^2}(\rho'\langle\rho\rangle_{,k} F_{,k} + \rho'\rho'_{,k} f'_{,k} + F_{,k}\rho'\rho'_{,k}). \end{aligned}$$

On the right-hand side of the equation, the largest term in the last two groups is $\rho'_{,k} f'_{,k}$ which is order $(\rho''/\langle\rho\rangle)^2$, so we neglect the other terms. The equation for F will be

$$F_{,t} + U_k F_{,k} + \langle u'_k f'_{,k}\rangle = \frac{d}{\langle\rho\rangle}\langle\rho'_{,k} f'_{,k}\rangle$$

and the equation for f'

$$f'_{,t} + u'_k F_{,k} + U_k f'_{,k} + u'_k f'_{,k} - \langle u'_k f'_{,k}\rangle = df'_{,kk} + \frac{d}{\langle\rho\rangle}(\rho'_{,\kappa} f'_{,k} - \langle\rho'_{,\kappa} f'_k\rangle).$$

If we note that

$$\langle u'_k f'_{,k}\rangle \approx \langle u'_k f'\rangle_{,k} + dc\langle\rho\rangle\langle f'_{,k} f'_{,k}\rangle \quad \text{and} \quad \langle\rho'_{,\kappa} f'_{,k}\rangle \approx -c\langle\rho\rangle^2\langle f'_{,k} f'_{,k}\rangle,$$

then we obtain

$$F_{,t} + U_k F_{,k} + \langle u'_k f'\rangle_{,k} = -2dc\langle\rho\rangle\langle f'_{,k} f'_{,k}\rangle. \tag{2.10}$$

The equation for f' is used for deriving the second-moment equation, and the pure mean term does not contribute, so for simplicity we suppress these terms and write

$$f'_{,t} + u'_k F_{,k} + U_k f'_{,k} + u'_k f'_{,k} = df'_{,kk} - dc\langle\rho\rangle f'_{,k} f'_{,k}. \tag{2.11}$$

From (2.3) we may write

$$\begin{aligned} U_{i,t} + u'_{i,t} + U_j U_{i,j} + u'_j U_{i,j} + U_j u'_{i,j} + u'_j u'_{i,j} \\ = -\frac{1}{\langle\rho\rangle}(P_{,i} + p'_{,i}) - c(P_{,i} f' + p'_{,i} f') + \nu(U_{i,j} + U_{j,i} + u'_{i,j} + u'_{j,i})_{,j} \\ + \nu c\langle\rho\rangle f'(U_{i,j} + U_{j,i} + u'_{i,j} + u'_{j,i})_{,j} + g_i, \end{aligned}$$

where ν is $\mu/\langle\rho\rangle$, $\rho'/\langle\rho\rangle \approx c\langle\rho\rangle f'$, and the term $\frac{2}{3}u_{p,p}$ has been neglected. The same argument as in the mass-fraction equation will lead to the following results:

$$U_{i,t} + U_j U_{i,j} + \langle u'_i u'_j\rangle_{,j} = -\frac{1}{\langle\rho\rangle}P_{,i} + g_i - c\langle\rho\rangle\left[\frac{1}{\langle\rho\rangle}\langle p'_{,i} f'\rangle + (\nu + d)\langle u'_{i,j} f'_{,j}\rangle\right], \tag{2.12}$$

$$\begin{aligned} u'_{i,t} + u'_j U_{i,j} + U_j u'_{i,j} + u'_j u'_{i,j} \\ = -\frac{1}{\langle\rho\rangle}p'_{,i} - c(P_{,i} f' + p'_{,i} f') + \nu(u'_{i,j} + u'_{j,i})_{,j} + \nu c\langle\rho\rangle f'(u'_{i,j} + u'_{j,i})_{,j}. \end{aligned} \tag{2.13}$$

Now we can use (2.11) and (2.13) to form the equations for the second moments, which are $\langle f'^2\rangle$, $\langle u_i' f'\rangle$, $\langle u_i' u_j'\rangle$. From (2.11) we may form

$$\langle f'^2\rangle_{,t}+U_k\langle f'^2\rangle_{,k}+2\langle u_k' f'\rangle F_{,k}+\langle u_k' f'^2_{,k}\rangle = 2d\langle f'f'_{,kk}\rangle-2dc\langle\rho\rangle\langle f'f'_{,k}f'_{,k}\rangle.$$

If we note that

$$\langle u_k' f'^2_{,k}\rangle \approx \langle u_k' f'^2\rangle_{,k}+2dc\langle\rho\rangle\langle f'f'_{,k}f'_{,k}\rangle \quad \text{and} \quad \langle f'f'_{,kk}\rangle \approx -\langle f'_{,k}f'_{,k}\rangle$$

for high Schmidt number, then we obtain an equation for $\langle f^2\rangle$:

$$\langle f'^2\rangle_{,t}+U_k\langle f'^2\rangle_{,k}+2\langle u_k' f'\rangle F_{,k}+\langle u'f'^2\rangle_{,k} = -2d\langle f'_{,k}f'_{,k}\rangle-4dc\langle\rho\rangle\langle f'f'_{,k}f'_{,k}\rangle. \tag{2.14}$$

From (2.11) and (2.13) we may form

$$\langle u_i' f'\rangle_{,t}+U_k\langle u_i' f'\rangle_{,k}+U_{i,k}\langle u_k' f'\rangle+F_{,k}\langle u_i' u_k'\rangle+\langle u_i' u_k' f'\rangle_{,k}$$
$$=-\frac{1}{\langle\rho\rangle}\langle p'_{,i}f'\rangle-(d+\nu)\langle u'_{i,k}f'_{,k}\rangle+c\langle\rho\rangle\left[-\frac{1}{\langle\rho\rangle}P_{,i}\langle f'^2\rangle-\frac{1}{\langle\rho\rangle}\langle p'_{,i}f'^2\rangle\right]. \tag{2.15}$$

From (2.13) we have

$$\langle u_i' u_j'\rangle_{,t}+U_k\langle u_i' u_j'\rangle_{,k}+U_{i,k}\langle u_j' u_k'\rangle+U_{j,k}\langle u_i' u_k'\rangle+\langle u_i' u_j' u_k'\rangle_{,k}$$
$$=-\frac{1}{\langle\rho\rangle}[\langle p'_{,i}u_j'\rangle+\langle p'_{,j}u_i'\rangle]-2\nu\langle u'_{i,k}u'_{j,k}\rangle$$
$$+c\langle\rho\rangle\left[-\frac{1}{\langle\rho\rangle}(P_{,i}\langle u_j' f'\rangle+P_{,j}\langle u_i' f'\rangle)-\frac{1}{\langle\rho\rangle}(\langle p'_{,j}u_i' f'\rangle+\langle p'_{,i}u_j' f'\rangle)\right]. \tag{2.16}$$

In (2.15) and (2.16) we have intensively used the assumption of high turbulent Reynolds number and high Schmidt number. The terms $\nu\langle u'_{i,k}u'_{i,k}\rangle$ and $d\langle f'_{,k}f'_{,k}\rangle$ are called the dissipation of turbulent energy and of variance of mass-fraction fluctuation. They are denoted by $\langle\epsilon\rangle$ and $\langle\epsilon_f\rangle$ respectively. As discussed, for example in Tennekes & Lumley (1972), the equations for these quantities (which can be obtained from (2.13) and (2.11) are not of much help; the production/destruction terms consist of small differences between large quantities, the latter written in dissipation range variables, but the differences being determined by energy-containing range variables. Essentially everything in the equation but the convection terms must be modelled. The results are

$$\langle\epsilon\rangle_{,t}+U_k\langle\epsilon\rangle_{,k}+\langle u_k'\epsilon'\rangle_{,k}=-\frac{\langle\epsilon\rangle^2}{q^2}\Psi, \tag{2.17}$$

$$\langle\epsilon_f\rangle_{,t}+U_k\langle\epsilon_f\rangle_{,k}+\langle u_k'\epsilon_f'\rangle_{,k}=-\frac{\langle\epsilon_f\rangle^2}{\langle f'^2\rangle}\Psi^f, \tag{2.18a}$$

where Ψ and Ψ^f contain all the production and destruction effects. We shall try to model Ψ and Ψ^f in a similar way to Lumley (1978).

Besides the above equations, we can easily obtain a continuity equation from (2.4):

$$\langle\rho\rangle_{,t}+(\langle\rho\rangle U_k-c\langle\rho\rangle^2\langle u_k' f'\rangle)_{,k}=0. \tag{2.18b}$$

From (2.18*b*) we see that in a two-dimensional statistically steady case it is convenient to introduce a mean stream function ψ, for example

$$\langle\rho\rangle U - c\langle\rho\rangle^2\langle u'f'\rangle = \frac{\partial\psi}{\partial y},$$

$$\langle\rho\rangle V - c\langle\rho\rangle^2\langle v'f'\rangle = -\frac{\partial\psi}{\partial x}.$$

So for future use, we rewrite all the equations in the following form:

$$L(F) + (\langle\rho\rangle\langle u_j'f'\rangle)_{,j} = c\langle\rho\rangle^2[-2\langle\epsilon_f\rangle - 2\langle u_j'f'\rangle F_{,j}], \tag{2.19}$$

$$L(U_i) + (\langle\rho\rangle\langle u_i'u_j'\rangle)_{,j} = -P_{,i} + \langle\rho\rangle g_i + c\langle\rho\rangle^2 \times\left[-\frac{1}{\langle\rho\rangle}\langle p'_{,i}f'\rangle - (\nu+d)\langle u'_{i,j}f'_{,j}\rangle - \langle u_j'f'\rangle U_{i,j} - \langle u_i'u_j'\rangle F_{,j}\right], \tag{2.20}$$

$$L(\langle f'^2\rangle) + 2\langle\rho\rangle\langle u_j'f'\rangle F_{,j} + (\langle\rho\rangle\langle u_j'f'^2\rangle)_{,j} = -2\langle\rho\rangle\langle\epsilon_f\rangle + c\langle\rho\rangle^2[-\langle u_j'f'\rangle\langle f'^2\rangle_{,j} - \langle u_j'f'^2\rangle F_{,j} - 4d\langle f'f'_{,j}f'_{,j}\rangle], \tag{2.21}$$

$$L(\langle u_i'f'\rangle) + \langle\rho\rangle\langle u_j'f'\rangle U_{i,j} + \langle\rho\rangle\langle u_i'u_j'\rangle F_{,j} + (\langle\rho\rangle\langle u_i'u_j'f'\rangle)_{,j} = -\langle p'_{,i}f'\rangle - \langle\rho\rangle(\nu+d)\langle u'_{i,j}f'_{,j}\rangle + c\langle\rho\rangle^2\left[-\frac{P_{,i}}{\langle\rho\rangle}\langle f'^2\rangle - \frac{1}{\langle\rho\rangle}p'_{,i}f'^2\rangle - \langle u_j'f'\rangle\langle u_i'f'\rangle_{,j} - \langle u_i'u_j'f'\rangle F_{,j}\right], \tag{2.22}$$

$$L(\langle u_i'u_j'\rangle) + \langle\rho\rangle\langle u_i'u_k'\rangle U_{j,k} + \langle\rho\rangle\langle u_j'u_k'\rangle U_{i,k} + (\langle\rho\rangle\langle u_i'u_j'u_k'\rangle)_{,k} = -(\langle p'_{,i}u_j'\rangle + \langle p'_{,j}u_i'\rangle) - 2\langle\rho\rangle\nu\langle u'_{i,k}u'_{j,k}\rangle + c\langle\rho\rangle^2\left[-\frac{1}{\langle\rho\rangle}(P_{,i}\langle u_j'f'\rangle + P_{,j}\langle u_i'f'\rangle) - \frac{1}{\langle\rho\rangle}(\langle p'_{,i}u_j'f'\rangle + \langle p'_{,j}u_i'f'\rangle) - \langle u_k'f'\rangle\langle u_i'u_j'\rangle_{,k} - \langle u_i'u_j'u_k'\rangle F_{,k}\right] \tag{2.23}$$

$$L(\langle\epsilon\rangle) + (\langle\rho\rangle\langle\epsilon'u_j'\rangle)_{,j} = -\langle\rho\rangle\frac{\langle\epsilon\rangle^2}{q^2}\Psi + c\langle\rho\rangle^2[-\langle u_j'f'\rangle\langle\epsilon\rangle_{,j} - \langle\epsilon'u_j'\rangle F_{,j}], \tag{2.24}$$

$$L(\langle\epsilon_f\rangle) + (\langle\rho\rangle\langle\epsilon_f'u_j'\rangle)_{,j} = -\langle\rho\rangle\frac{\langle\epsilon_f\rangle^2}{\langle f'^2\rangle}\Psi^f + c\langle\rho\rangle^2[-\langle u_j'f'\rangle\langle\epsilon_f\rangle_{,j} - \langle\epsilon_f'u'\rangle F_{,j}], \tag{2.25}$$

where $L(\ ) \equiv \langle\rho\rangle(\ )_{,t} + (\langle\rho\rangle U_j - c\langle\rho\rangle^2\langle u_j'f'\rangle)(\ )_{,j}$.

Equations (2.19)–(2.25) are the general basic equations for variable-density flows (mixing fluids) on the assumptions of high turbulent Reynolds and Schmidt number and small ratio of $\rho''/\langle\rho\rangle$. The effects of variable density are represented by terms with the factor c. If we let $c = 0$, then the equations will reduce to constant-density flow with a passive scalar. It is interesting to note the appearance of the mean-pressure gradient in the varible-density terms of the second-moment equation. We may expect that the effects of the pressure gradient will be stronger in variable-density flow than in constant-density flow. These equations are evidently not closed; many terms must be modelled. There are basically four types of terms:

(i) third moments, like $\langle u_i'u_j'u_k'\rangle$, $\langle u_i'u_j'f'\rangle$, $\langle u_j'f'^2\rangle$;
(ii) pressure correlations, like $\langle p'_{,i}u_j'\rangle$, $\langle p'_{,i}f'\rangle$;
(iii) more complicated terms, $d\langle f'f'_{,k}f'_{,k}\rangle$, $\langle p'_{,j}f'^2\rangle$, $\langle p'_{,i}u_j'f'\rangle$;
(iv) the terms in the dissipation equation, $\langle u_j'\epsilon'\rangle$, $\langle u_j'\epsilon_f'\rangle$, Ψ, Ψ^f.

For the terms of type (i) and (iii), we use a zeroth-order (constant-density) approximation of the third-moment equations to obtain expressions for the third moments and the more complicated terms. For the terms of type (ii), we shall follow the procedure for constant-density flow and use Poisson's equation for the pressure fluctuation and realizability to propose several possible models. The model terms in the dissipation equations, $\langle u_j' \epsilon' \rangle$, $\langle u_j' \epsilon_f' \rangle$, are taken from Lumley (1978). Ψ and Ψ^f are formed in a new way based on the equilibrium value of the timescale ratio (the ratio of the mechanical timescale to the scalar timescale).

3. Modelling

3.1. *Models for third moments and more complicated terms*

The zeroth-order approximation for the third moments is obtained by a perturbation expansion about a (Gaussian) equilibrium state in the homogeneous limit for a constant-density flow (Lumley 1978). The method is somewhat reminiscent of non-equilibrium thermodynamics of mixtures, with the various second-order quantities playing the role of the species. This approach is essentially unique in modelling, in being based on first principles, and does not introduce adjustable constants. Janicka & Lumley (1981) showed that for a variable-density flow, this basic approach is also satisfactory, and the influence of the variable density on the third-moment equations appears only at a higher-order level, $(\rho''/\langle\rho\rangle)^2$. Therefore, the models of the third moments for a constant-density flow can be used in a variable-density flow. Here is the list of models for the third moments (Lumley 1978):

$$\langle u_j' f'^2 \rangle = -[\langle f'^2 \rangle_{,k} \langle u_j' u_k' \rangle + 2\langle u_j' f' \rangle_{,k} \langle u_k' f' \rangle] \frac{\langle \epsilon \rangle / 2\langle q^2 \rangle}{r + \Phi^f}, \tag{3.1}$$

$$\langle u_i' u_j' f' \rangle = \Big(-[\langle u_i' f' \rangle_{,k} \langle u_k' u_j' \rangle + \langle u_j' f' \rangle_{,k} \langle u_k' u_i' \rangle + \langle u_i' u_j' \rangle_{,k} \langle u_k' f' \rangle] + \tfrac{1}{3}(\beta - 2) \frac{\langle \epsilon \rangle}{q^2} \langle q'^2 f' \rangle \delta_{ij} \Big) \frac{q^2/\langle \epsilon \rangle}{\beta + 2\Phi^f}, \tag{3.2}$$

$$\langle u_i' u_j' u_k' \rangle = \frac{1}{3\beta} \frac{q^2}{\langle \epsilon \rangle} \Big(-[\langle u_i' u_j' \rangle_{,p} \langle u_k' u_p' \rangle + \langle u_i' u_k' \rangle_{,p} \langle u_j' u_p' \rangle + \langle u_j' u_k' \rangle_{,p} \langle u_i' u_p' \rangle] + \tfrac{1}{3}(\beta - 2) \frac{\langle \epsilon \rangle}{q^2} (\delta_{ij} \langle q^2 u_k' \rangle + \delta_{ik} \langle q^2 u_j' \rangle + \delta_{jk} \langle q^2 u_i' \rangle) \Big), \tag{3.3}$$

where
$$\langle q^2 f' \rangle = -\frac{1}{2} \frac{q^2}{\langle \epsilon \rangle} \frac{2\langle u_i' f' \rangle_{,k} \langle u_k' u_i' \rangle + q^2_{,k} \langle u_k' f' \rangle}{1 + \Phi^f}, \tag{3.4}$$

$$\langle q^2 u_\kappa' \rangle = -3 \frac{q^2}{\langle \epsilon \rangle} \frac{q^2_{,p} \langle u_k' u_p' \rangle + 2\langle u_i' u_k' \rangle_{,p} \langle u_i' u_p' \rangle}{4\beta + 10}, \tag{3.5}$$

and β, Φ^f, will be presented later.

For the 'more complicated' terms of type (3), first we write the equations for the third moments making use of the results of the perturbation expansion to eliminate fourth cumulants and time derivatives but keeping pressure correlations and viscous terms in their primitive form. We need in particular $\langle f'^3 \rangle$, $\langle u_i' f'^2 \rangle$ and $\langle u_i' u_j' f' \rangle$. We keep only zeroth-order terms in $\rho''/\langle\rho\rangle$, and assume high Reynolds and/or Schmidt number to omit all the terms that contain the diffusivity d and viscosity μ, except the term $d\langle f'f'_{,j}f'_{,j}\rangle$ in the equation of $\langle f'^3\rangle$, which is $\langle f'\epsilon'_f\rangle$ and should be modelled. We obtain:

from the equation of $\langle f'^3\rangle$,

$$\langle u'_j f'\rangle \langle f'^2\rangle_{,j} = -2d\langle f'f'_{,j}f'_{,j}\rangle; \tag{3.6}$$

from the equation of $\langle u'_i f'^2\rangle$,

$$\langle u'_k u'_i\rangle \langle f'^2\rangle_{,k} + 2\langle u'_k f'\rangle \langle u'_i f'\rangle_{,k} = -\frac{1}{\langle\rho\rangle}\langle p'_{,i} f'^2\rangle; \tag{3.7}$$

from the equation of $\langle u'_i u'_j f'\rangle$,

$$\langle u'_k u'_i\rangle \langle u'_j f'\rangle_{,k} + \langle u'_k u'_j\rangle \langle u'_i f'\rangle_{,k} + \langle u'_k f'\rangle \langle u'_i u'_j\rangle_{,k} = -\frac{1}{\langle\rho\rangle}\langle p'_{,j} u'_i f'\rangle + \langle p'_{,i} u'_j f'\rangle); \tag{3.8}$$

and these are the required terms.

3.2. *Models for* $\langle u'\epsilon'\rangle$, $\langle u'\epsilon_f\rangle$, Ψ *and* Ψ^f

The models for the dissipation equation are the weakest point of second-order modelling. Equations (2.17) and (2.18) are formally of the same form as for constant-density flow. As we discussed in §3.1, the effects of variable density on the transport terms are of order $(\rho''/\rho)^2$, and hence are negligible. We can thus expect to use the constant-density form for $\langle u'_k \epsilon\rangle$ and $\langle u'_j \epsilon_f\rangle$. For Ψ and Ψ^f, we shall try a new form which causes the timescale ratio (the ratio of mechanical to scalar timescale) to relax toward an equilibrium value at a rate that differs depending on whether the timescale ratio is greater or less than the equilibrium value, and which depends on the distance from the equilibrium value. A version of this has been exercised in atmospheric calculations by P. Mansfield (private communication) with satisfactory results.

Here we list these models:

$$\langle u'_k \epsilon\rangle = -\frac{9}{5}\frac{q^2}{\langle\epsilon\rangle}\frac{[\langle u'_k u'_p\rangle + 2\langle u'_i u'_k\rangle \langle u'_p u'_i\rangle/q^2]\langle\epsilon\rangle_{,p}}{4\beta+10}; \tag{3.9}$$

$$\langle u'_j \epsilon_f\rangle = -0.5\frac{\langle\epsilon\rangle}{q^2}\frac{[\langle u'_k u'_j\rangle + \langle u'_j f'\rangle \langle u'_k f'\rangle/\langle f'^2\rangle]\langle\epsilon_f\rangle_{,k}}{r+\Phi^f}; \tag{3.10}$$

$$\Psi = \Psi_0 + \frac{\Psi_1 b_{ij} q^2 U_{i,j}}{\langle\epsilon\rangle}; \tag{3.11}$$

$$\Psi^f = \Psi^f_0 + \frac{\Psi^f_1 \langle u'_i f'\rangle F_{,i}}{\langle\epsilon_f\rangle}; \tag{3.12}$$

where

$$\Psi_0 = \tfrac{14}{5} + 0.98\exp\left(\frac{-2.83}{R_l^{\frac{1}{2}}}\right)[1-0.33\ln(1-55\mathrm{II})],$$

$$\Psi_1 \approx 2.0-2.4$$

$$\Psi^f_0 = 2 - \frac{2-\Psi_0}{r} + b(-\mathrm{II})^a\frac{(r/r_e-1)^c}{r}$$

$$\Psi^f_1 = \left(2+\frac{\Psi_1-2}{r_e}\right)\left(\frac{r_e}{r}\right)^d \quad \text{if } r < r_e$$

or $$= \left(2+\frac{\Psi_1-2}{r_e}\right)\left[1-A\left(1-\frac{r_e}{r}\right)\right] \quad \text{if } r > r_e$$

and $$a = 1, \quad b = 3, \quad c = 1, \quad d = 10, \quad A = 0.1,$$

$$r_e = 1.55, \quad r \equiv \left(\frac{q^2}{\langle\epsilon\rangle}\right)\Big/\left(\frac{\langle f'^2\rangle}{\langle\epsilon_f\rangle}\right),$$

$$\mathrm{II} = -\tfrac{1}{2}\mathrm{b}_{ij}\,\mathrm{b}_{ji}, \quad \mathrm{b}_{ij} = \frac{\langle u_i' u_j'\rangle}{q^2} - \tfrac{1}{3}\delta_{ij}.$$

3.3. *Pressure fluctuation*

The standard procedure for modelling the correlations between pressure gradient and velocity or a scalar is first to study the behaviour of the pressure fluctuations. We may obtain the Poisson equation for the instantaneous pressure from (2.3) as follows:

$$-p_{,ii} = -\tfrac{4}{3}\mu(u_{i,i})_{,jj} + \frac{\rho \mathrm{D}}{\mathrm{D}t}(u_{i,i}) + \rho_{,i}\frac{\mathrm{D}}{\mathrm{D}t}(u_i) + \rho u_{i,j}u_{j,i}$$

where $\mathrm{D}/\mathrm{D}t$ stands for $(\;)_{,t} + u_j(\;)_{,j}$. In a constant-density flow, the first three terms on the right-hand side of the equation will disappear. They represent the principle effects of variable density on the pressure. In the case of a mixture, we may write, from (2.11), (2.2) and (2.4),

$$u_{i,i} = -\frac{1}{\rho}\frac{\mathrm{D}\rho}{\mathrm{D}t} = c\rho\frac{\mathrm{D}f}{\mathrm{D}t} = dc(\rho f_{,i})_{,i}.$$

Substituting this into the pressure equation gives

$$\underset{(1)}{-p_{,ii} = -\tfrac{4}{3}\mu dc(\rho f_{,i})_{,ijj}} + \underset{(2)}{dc\rho\frac{\mathrm{D}}{\mathrm{D}T}(\rho f_{,i})_{,i}} - \underset{(3)}{c\rho^2 f_{,i}\frac{\mathrm{D}}{\mathrm{D}t}(u_i)} + \underset{(4)}{\rho u_{i,j}u_{j,i}}.$$

We are dealing here with instantaneous variables – mean plus fluctuation. To get a rough idea of orders of magnitude, consider a general laminar flow, and take $u_{i,j} \approx O(u/l)$, $f_{,i} \approx O(\Delta f/l)$ and $\mathrm{D}u_i/\mathrm{D}t \approx O(u^2/l)$, where l is the smallest of the lengthscales in the various directions. The relative order of magnitude of the various terms on the right-hand side of the equation will be

$$\underset{(1)}{c\rho\Delta f\frac{\nu}{ul}\frac{d}{ul}}, \quad \underset{(2)}{c\rho\Delta f\frac{d}{ul}}, \quad \underset{(3)}{c\rho\Delta f}, \quad \underset{(4)}{1}.$$

Therefore, the first two terms can be made as small as we like by making the Reynolds/Schmidt number sufficiently high. The third term is of order $c\rho\Delta f$, which is the main effect of variable density on the pressure. Note that this analysis is on a sound footing only for a mixing (non-exothermic) flow. With heat release, the terms in $u_{i,i}$ can be of much larger order. Now if we decompose the instantaneous quantities into their mean and fluctuating parts (see (2.5)), we may write

$$-p'_{,ii} = 2\langle\rho\rangle\, U_{i,j}u'_{j,i} + \langle\rho\rangle\, u'_{i,j}u'_{j,i} + O(c\langle\rho\rangle f').$$

In this equation the first two terms are identical with the constant-density case, and the remaining terms are of order $c\langle\rho\rangle f'$ (which represents the effects of variable density). Now let us estimate at what order of magnitude these first-order $(c\langle\rho\rangle f')$

terms affect the pressure correlations in (2.19)–(2.25). First, in the mean-velocity equation, these terms will appear as second-order terms $(c\langle\rho\rangle f'')^2$, because there is a factor of order $c\langle\rho\rangle f''$ in front of the pressure correlation. Secondly, in the second-moment equations, they will appear to first order $c\langle\rho\rangle f''$. However, in our gas mixing layer (thin-shear-layer flow), we shall see (in §4) that $c\langle\rho\rangle f'' \approx O(l/L)^{\frac{1}{2}}$. If we discard terms of order $(l/L)^{\frac{1}{2}}$ in the second-moment equations (as we shall), we may also neglect the effects of variable density on the pressure correlations. We shall consequently use more-or-less familiar constant-density forms for all the pressure correlations, and consistently neglect the divergence of velocity (which can be considered as a diffusivity term, see (2.9)). We shall give derivations *in extenso* only when we have somewhat elaborated the traditional models. We may now write

$$-p'_{,ii} = 2\langle\rho\rangle U_{i,j} u'_{j,i} + \langle\rho\rangle u'_{i,j} u'_{j,i}. \tag{3.13}$$

Because of the linearity of this equation, we may split it into two parts as follows:

$$-p'_{\mathrm{ra},ii} = 2\langle\rho\rangle U_{i,j} u'_{j,i}, \tag{3.14}$$

$$-p'_{\mathrm{re},ii} = \langle\rho\rangle u'_{i,j} u'_{j,i}, \tag{3.15}$$

and write

$$p' = p'_{\mathrm{ra}} + p'_{\mathrm{re}} \tag{3.16}$$

The correlations containing p'_{ra}, and p'_{re}, are called the rapid term, and the return term respectively. The total pressure correlation can be written in the following way:

$$\langle p'_{,i} u'_j\rangle = \langle p'_{\mathrm{ra},i} u'_j\rangle + \langle p'_{\mathrm{re},i} u'\rangle, \tag{3.17}$$

$$\langle p'_{,i} f\rangle = \langle p'_{\mathrm{ra},i} f'\rangle + \langle p'_{\mathrm{re},i} f'\rangle. \tag{3.18}$$

3.4. *Model of* $\langle p'_{,i} u'_j\rangle$

$\langle p'_{\mathrm{re},i} u'_j\rangle$

We may re-write this term as follows:

$$\langle p'_{\mathrm{re},i} u'_j\rangle = \langle p'_{\mathrm{re}} u'_j\rangle_{,i} - \langle p'_{\mathrm{re}} u'_{j,i}\rangle.$$

The first term on right-hand side of this equation is called the pressure transport term. We model this in the same way as Lumley (1978), but correct an error made there. Lumley (1978) did not consider the most general linear expression; if we add the term he neglected we obtain

$$\langle p'_{\mathrm{re}} u'_k\rangle = -C\langle\rho\rangle\langle q^2 u'_k\rangle, \tag{3.19}$$

where C is an undetermined coefficient, rather than the fixed value of 0.2 which he obtained. We shall derive the corresponding scalar quantity in §3.5.

Now let us consider the model of $\langle p'_{\mathrm{re}} u'_{j,i}\rangle$. This term is usually called 'the return to isotropy'. The molecular term, $\nu\langle u'_{i,k} u'_{j,k}\rangle$, also plays a part in the return to isotropy. We model them together and define a tensor Φ_{ij} as follows:

$$-\Phi_{ij}\langle\epsilon\rangle = \frac{1}{\rho}\langle p'_{\mathrm{re}}(u'_{i,j} + u'_{j,i})\rangle - 2\nu\langle u'_{i,k} u'_{j,k}\rangle + \tfrac{2}{3}\langle\epsilon\rangle\delta_{ij}. \tag{3.20}$$

The arguments by Lumley (1978) lead to the following model for Φ:

$$\left.\begin{aligned} \Phi_{ij} &= \beta b_{ij}, \\ b_{ij} &= \frac{\langle u'_i u'_j\rangle}{q^2} - \tfrac{1}{3}\delta_{ij}, \end{aligned}\right\} \tag{3.21}$$

where β is a function of the turbulent Reynolds number and invariants of b_{ij},

$$\beta = 2+\exp\left(-\frac{D}{R_l^{\frac{1}{2}}}\right)\left[\frac{72}{R_l^{\frac{1}{2}}}+A\ \ln\left(1+B(-\mathrm{II}+C\mathrm{III})\right)\right]\left[\tfrac{1}{9}+3\mathrm{III}+\mathrm{II}\right], \quad (3.22)$$

$$\mathrm{II} = -\tfrac{1}{2}b_{ij}\,b_{ij}, \quad \mathrm{III} = \tfrac{1}{3}b_{ij}\,b_{jk}\,b_{ki},$$

$$A = 80.1, \quad B = 62.4, \quad C = 2.3, \quad D = 7.77.$$

$\langle p'_{\mathrm{ra},j}\,u'_j\rangle$

This term, which contains the mean-velocity gradient, is usually called the rapid term. In the usual way, we may form from (3.14)

$$\langle p'_{\mathrm{ra},j}\,u'_i\rangle = 2\langle\rho\rangle\,U_{p,q}\,\frac{1}{4\pi}\iiint_v \langle u'_q(\boldsymbol{r})\,u'_i(\boldsymbol{r}')\rangle_{,r_p r_j}\frac{\mathrm{d}v}{|\boldsymbol{r}-\boldsymbol{r}'|}$$

supposing (in the usual quasi-homogeneous approximation) that the scale of variation of the mean-density and mean-velocity gradient is large relative to the scale of the double correlation, permitting the former to be removed from the integral.

Now if we define a tensor $\boldsymbol{X}$ as

$$X^{qi}_{pj} = -\frac{1}{4\pi}\iiint\langle u'_q(\boldsymbol{r})\,u'_i(\boldsymbol{r}')\rangle_{,r_p r_j}\frac{\mathrm{d}v}{|\boldsymbol{r}-\boldsymbol{r}'|} \quad (3.23)$$

then we have

$$\langle p'_{\mathrm{ra},j}\,u'_i\rangle = -2\langle\rho\rangle\,U_{p,q}\,X^{qi}_{pj}. \quad (3.24)$$

From (3.23), $\boldsymbol{X}$ has the following properties:

(a) $X^{qi}_{pj} = X^{iq}_{pj}, \quad X^{qi}_{pj} = X^{qi}_{jp}$,
(b) $X^{qi}_{pp} = \langle u'_q\,u'_i\rangle$,
(c) $X^{qj}_{pj} \approx 0$,

where (c) is an approximation, since we are neglecting the divergence of the velocity fluctuations in the correlation. If we assume that $\boldsymbol{X}$ is a linear combination of b_{ij}, then these properties will lead to the classical model (Launder, Reece & Rodi 1975)

$$X^{qi}_{pj} = -\frac{q^2}{3}(b_{pj}\,\delta_{qi}-\delta_{pj}\,b_{qi})+\frac{q^2}{30}(4\delta_{pj}\,\delta_{qi}-\delta_{pq}\,\delta_{ij}-\delta_{pi}\,\delta_{qj})$$
$$+Cq^2(b_{pq}\,\delta_{ij}+b_{jq}\,\delta_{ip}+b_{pi}\,\delta_{qj}+b_{ij}\,\delta_{pq}-\tfrac{11}{3}b_{pj}\,\delta_{qi}-\tfrac{4}{3}\delta_{pj}\,b_{qi}), \quad (3.25)$$

where C is a constant, $C = -0.166$ in a constant-density flow. This model form does not satisfy the realizability consideration raised by Lumley (1978). Here we suggest a new form (see Shih 1984) which contains higher-order tensors in b_{ij}, and which satisfies realizability exactly:

$$X^{qi}_{pj} = -\frac{q^2}{3}(\delta_{qi}\,b_{pj}-\delta_{pj}\,b_{qi})+\frac{q^2}{30}(4\delta_{pj}\,\delta_{qi}-\delta_{pq}\,\delta_{ij}-\delta_{pi}\,\delta_{qj})$$
$$-\frac{q^2}{10}(\delta_{pq}\,b_{ij}+\delta_{ij}\,b_{pq}+\delta_{qj}\,b_{pi}+\delta_{pi}\,b_{qj}-\tfrac{11}{3}\delta_{qi}\,b_{pj}-\tfrac{4}{3}\delta_{pj}\,b_{qi})$$
$$+\frac{q^2}{10}(2\delta_{pj}\,b^2_{qi}-3b_{pq}\,b_{ij}-3b_{qj}\,b_{pi}+b_{qi}\,b_{pj}). \quad (3.26)$$

3.5. *Model of* $\langle p'_{,i} f' \rangle$

Now let us discuss the correlations between the pressure gradient and scalar. We shall follow the same procedure as we used for the correlations between pressure gradient and velocity.

$\langle p'_{\mathrm{re},i} f' \rangle$

This term can be split into two parts: $\langle p'_{\mathrm{re}} f' \rangle_{,i} - \langle p'_{\mathrm{re}} f'_{,i} \rangle$. First we discuss the 'pressure transport' term, $\langle p'_{\mathrm{re}} f' \rangle$. As discussed in Lumley (1978), this term is, of course, not a transport term as usually defined, but appears to be required for consistency. Since a form for this term was not derived in Lumley (1978), we shall derive it here. From (3.15) we may form

$$\langle p'_{\mathrm{re}} f' \rangle = \langle \rho \rangle \frac{1}{4\pi} \iiint_v \langle u'_i u'_j(\boldsymbol{r}) f'(\boldsymbol{r}') \rangle_{,r_i r_j} \mathrm{d}v / |\boldsymbol{r} - \boldsymbol{r}'|. \tag{3.27}$$

If we define the following tensor:

$$Y^{ij}_{pq} = -\frac{1}{4\pi} \iiint_v \langle u'_i u'_j(\boldsymbol{r}') f'(\boldsymbol{r}') \rangle_{,r_p r_q} \mathrm{d}v / |\boldsymbol{r} - \boldsymbol{r}'|, \tag{3.28}$$

then

$$\langle p'_{\mathrm{re}} f' \rangle = -\langle \rho \rangle Y^{ij}_{ij}. \tag{3.29}$$

Equation (3.28) shows that this tensor has the following properties:

(*a*) $Y^{ij}_{pq} = Y^{ji}_{pq}, \quad Y^{ij}_{pq} = Y^{ij}_{qp}$,

(*b*) $Y^{ij}_{pp} = \langle u'_i u'_j f' \rangle$.

If we assume that this tensor is a linear function of $\langle u'_i u'_j f' \rangle$ (written as r_{ij}), then we may form

$$Y^{ij}_{pq} = \alpha_1 \delta_{pq} r_{ij} + \alpha_2 \delta_{ij} r_{pq} + \alpha_3(\delta_{pi} r_{jq} + \delta_{pj} r_{iq} + \delta_{qi} r_{jp} + \delta_{qj} r_{ip}) + \alpha_4 \delta_{ij} \delta_{pq} r_{kk} + \alpha_5(\delta_{ip}\delta_{jq} + \delta_{iq}\delta_{jp}) r_{kk},$$

which already satisfies (*a*). Condition (*b*) and (3.29) will lead to the following form with an undetermined coefficient C which is a combination of α's:

$$\langle p'_{\mathrm{re}} f' \rangle = -C \langle \rho \rangle \langle q^2 f' \rangle.$$

As discussed in Lumley (1978), this should have the same value as C in (3.19).

The return term $\langle p'_{\mathrm{re}} f'_{k} \rangle$ has been discussed by Shih & Lumley (1986), that is

$$\langle p'_{\mathrm{re}} f'_{,k} \rangle = -\langle \rho \rangle \Phi^f \langle u'_k f' \rangle \frac{\langle \epsilon \rangle}{q^2}, \tag{3.30}$$

$$\Phi^f = \tfrac{1}{2}\beta + r - \frac{\frac{1}{2}(\beta - 2) Q}{P + Q} + 1 \cdot 1 r^2 F^{\frac{1}{2}}_D, \tag{3.31}$$

$$Q = \tfrac{1}{6}(1 - D^2_{ii}),$$

$$P = D_{ij} b_{jk} D_{ki} - b_{ij} D_{ij}),$$

$$F_D = 9 D^3_{ii} - \tfrac{27}{2} D^2_{ii} + \tfrac{9}{2},$$

$$D_{ij} = \frac{\langle f'^2 \rangle \langle u'_i u'_j \rangle - \langle u'_i f' \rangle \langle u'_j f' \rangle}{\langle f'^2 \rangle q^2 - \langle u'_p f' \rangle \langle u'_p f' \rangle},$$

$$r \equiv \frac{q^2}{\langle \epsilon \rangle} \frac{\langle \epsilon_f \rangle}{\langle f'^2 \rangle}.$$

$\langle p'_{\mathrm{ra},k} f' \rangle$

This rapid term in the scalar flux equation can be shown to be

$$\langle p'_{\mathrm{ra},k} f' \rangle = -2\langle \rho \rangle U_{j,i} X^i_{kj}, \tag{3.32}$$

where the tensor $\boldsymbol{X}$ is defined by

$$X^i_{kj} = -\frac{1}{4\pi} \iiint_v \langle f'(\boldsymbol{r})\, u'_i(\boldsymbol{r}') \rangle_{,r_k r_j} \mathrm{d}v/|\boldsymbol{r}-\boldsymbol{r}'|. \tag{3.33}$$

Obviously, we shall obtain the following conditions from (3.33):

(a) $X^i_{kj} = X^i_{jk}$,

(b) $X^i_{jj} = \langle u'_i f' \rangle$,

(c) $X^j_{kj} \approx 0$.

Now if we assume that the tensor $\boldsymbol{X}$ is only a function of $\langle u'_i f' \rangle$ and b_{ij}, then a general form is

$$X^i_{jk} = \beta_1 \delta_{jk}\langle fu_i \rangle + \beta_2(\delta_{ij}\langle fu_k \rangle + \delta_{ik}\langle fu_j \rangle) + \beta_3 b_{jk}\langle fu_i \rangle + \beta_4(b_{ij}\langle fu_k \rangle + b_{ik}\langle fu_j \rangle) + \beta_5(\delta_{ij} b_{kp} + \delta_{ki} b_{jp})\langle fu_p \rangle + \beta_6 \delta_{jk} b_{ip}\langle fu_p \rangle,$$

which already satisfies condition (a). From conditions (b), (c) and the realizability condition suggested by Lumley (1978), we obtain a new form (also see Shih 1984):

$$X^i_{kj} = \tfrac{2}{5}\delta_{jk}\langle fu_i \rangle - \tfrac{1}{10}(\delta_{ik}\langle fu_j \rangle + \delta_{ij}\langle fu_k \rangle) + \tfrac{1}{10} b_{jk}\langle fu_i \rangle - \tfrac{3}{10}(b_{ik}\langle fu_j \rangle + b_{ij}\langle fu_k \rangle) + \tfrac{1}{5}\delta_{jk} b_{ip}\langle fu_p \rangle. \tag{3.34}$$

Note that the first two terms of this form have been used by most authors, but do not satisfy realizability.

4. The simplified equations

The flows considered here are almost parallel, two-dimensional flows for which the boundary-layer approximation is applicable. For these flows it is possible to simplify the equations for the second moments (say, Reynolds stress and scalar flux) by neglecting small terms. To identify these terms, we must determine in what order the terms vanish as these flows become more and more parallel. We shall concentrate on mixing-layer flow (the shear layer). Other types of flows (jets, wakes and axisymmetric flows) can be analysed in the same way. For the mixing layer there are two velocity scales: U_s for the cross-stream variation of the mean velocity component in the x-direction; u for the velocity scale of the turbulence. We introduce temporarily a scale V_s for the mean cross-stream velocity component. In addition, there are two lengthscales: L for the scale of change in the x-direction; l for the scale of change in the y-direction. For the scalar quantities, we define F_s and f_s as the scales of the mean mass fractions and the mass-fraction fluctuations respectively. According to the above, we may write $\partial\langle \rho \rangle U/\partial x = O(\langle \rho \rangle U_s/L)$, $\partial\langle \rho \rangle U/\partial y = O(\langle \rho \rangle U_s/l)$, $\partial\langle \rho \rangle V/\partial y = O(\langle \rho \rangle V_s/l)$, $\langle uv \rangle = O(u^2)$, $\langle u^2 \rangle = O(u^2)$, $\langle v^2 \rangle = O(u^2)$ etc, where $O(\ )$ stands for 'order of magnitude'.

Now let us consider the mean continuity equation:

$$\frac{\partial\langle \rho \rangle U}{\partial x} + \frac{\partial\langle \rho \rangle V}{\partial y} - \frac{\partial(c\langle \rho \rangle^2 \langle uf \rangle)}{\partial x} - \frac{\partial(c\langle \rho \rangle^2 \langle vf \rangle)}{\partial y} = 0 \tag{4.1}$$

$$O(1) \quad O\left(\frac{V_s}{U_s}\frac{L}{l}\right) \quad O\left(c\langle \rho \rangle f_s \frac{u}{U_s}\right) \quad O\left(c\langle \rho \rangle f_s \frac{u}{U_s}\frac{L}{l}\right)$$

Listed underneath (4.1) are the relative orders of magnitude of each term in (4.1). The third term is obviously vanishingly small compared with the fourth term in the limit as $l/L \to 0$; hence the fourth term is the only 'correction' term for density fluctuations. For the worst case, that the 'correction' term for density is as large as others in (4.1), we must require

$$V_s = O\left(\frac{U_s l}{L}\right), \tag{4.2}$$

$$c\langle\rho\rangle f_s = O\left(\frac{U_s}{u}\frac{l}{L}\right). \tag{4.3}$$

The mean continuity equation becomes

$$\frac{\partial\langle\rho\rangle U}{\partial x} + \frac{\partial(\langle\rho\rangle V - c\langle\rho\rangle^2\langle vf\rangle)}{\partial y} = 0. \tag{4.4}$$

The equation for U reads

$$\langle\rho\rangle U\frac{\partial U}{\partial x} + (\langle\rho\rangle V - c\langle\rho\rangle^2\langle vf\rangle)\frac{\partial U}{\partial y} + \frac{\partial\langle\rho\rangle\langle u^2\rangle}{\partial x} + \frac{\partial\langle\rho\rangle\langle uv\rangle}{\partial y}$$

$$O\left(\frac{\langle\rho\rangle U_s^2}{L}\right) \qquad O\left(\frac{\langle\rho\rangle u^2}{L}\right) \quad O\left(\frac{\langle\rho\rangle u^2}{l}\right)$$

$$= c\langle\rho\rangle^2\left(\ldots - \langle uf\rangle\frac{\partial U}{\partial x} - \langle vf\rangle\frac{\partial U}{\partial y} - \langle u^2\rangle\frac{\partial F}{\partial x} - \langle uv\rangle\frac{\partial F}{\partial y}\right). \tag{4.5}$$

$$O\left(\frac{uf_s U_s}{L}\right) \quad O\left(\frac{uf_s U_s}{l}\right) \quad O\left(\frac{u^2 F_s}{L}\right) \quad O\left(\frac{u^2 F_s}{l}\right)$$

Again the terms of $\partial\langle\rho\rangle\langle u^2\rangle/\partial x$, $\langle uf\rangle\partial U/\partial x$ and $\langle u^2\rangle\partial F/\partial x$ can be neglected compared to $\partial\langle\rho\rangle\langle uv\rangle/\partial y$, $\langle vf\rangle\partial U/\partial y$ and $\langle uv\rangle\partial F/\partial y$, in the limit as $l/L \to 0$, and the following relations must hold if all the remaining terms are of the same order of magnitude:

$$\frac{u}{U_s} = O\left(\frac{l}{L}\right)^{\frac{1}{2}}, \tag{4.6}$$

$$c\langle\rho\rangle F_s = O\left(\frac{c\langle\rho\rangle f_s U_s}{u}\right). \tag{4.7}$$

From (4.3) and (4.6) we obtain

$$c\langle\rho\rangle f_s = O\left(\frac{l}{L}\right)^{\frac{1}{2}}; \tag{4.8}$$

hence

$$c\langle\rho\rangle F_s = O(1). \tag{4.9}$$

The equation for U becomes

$$\langle\rho\rangle U\frac{\partial U}{\partial x} + (\langle\rho\rangle V - c\langle\rho\rangle^2\langle vf\rangle)\frac{\partial U}{\partial y} + \frac{\partial\langle\rho\rangle\langle uv\rangle}{\partial y}$$

$$= c\langle\rho\rangle^2\left[-\frac{1}{\langle\rho\rangle}\langle p_{,x}f\rangle - (\nu + d)\langle u_{,j}f_{,j}\rangle - \langle vf\rangle\frac{\partial U}{\partial y} - \langle uv\rangle\frac{\partial F}{\partial y}\right]. \tag{4.10}$$

In a similar way we shall obtain the equation for F:

$$\langle\rho\rangle U\frac{\partial F}{\partial x} + (\langle\rho\rangle V - c\langle\rho\rangle^2\langle vf\rangle)\frac{\partial F}{\partial y} + \frac{\partial\langle\rho\rangle\langle vf\rangle}{\partial y} = c\langle\rho\rangle^2\left[-2\epsilon_f - 2\langle vf\rangle\frac{\partial F}{\partial y}\right]. \tag{4.11}$$

The equation for $\langle uv\rangle$ reads

$$\langle\rho\rangle\, U\frac{\partial\langle uv\rangle}{\partial x}+(\langle\rho\rangle\, V-c\langle\rho\rangle^{2}\langle vf\rangle)\frac{\partial\langle uv\rangle}{\partial y}+\langle\rho\rangle\langle uv\rangle\frac{\partial V}{\partial y}+\langle\rho\rangle\langle v^{2}\rangle\frac{\partial U}{\partial y}$$
$$\text{(1)}\qquad\qquad\text{(2)}\qquad\qquad\text{(3)}\qquad\qquad\text{(4)}$$
$$+\frac{\partial(\langle\rho\rangle\langle uv^{2}\rangle-0.2\langle\rho\rangle\langle q^{2}u\rangle)}{\partial y}$$
$$\text{(5)}$$
$$=\ldots+c\langle\rho\rangle^{2}\left[-\langle uv^{2}\rangle\frac{\partial F}{\partial y}+\langle uv\rangle\frac{\partial\langle vf\rangle}{\partial y}+\langle v^{2}\rangle\frac{\partial\langle uf\rangle}{\partial y}\right]. \tag{4.12}$$
$$\text{(6)}\qquad\qquad\text{(7)}$$

Where '...' stands for the pressure and dissipation terms. The order of magnitude of each term in (4.12) is as follows:

$$(1)=O\left(A\frac{l}{L}\right),\quad \text{where } A\equiv\frac{\langle\rho\rangle\, u^{2}U_{\mathrm{s}}}{l},$$
$$(2)=O\left(A\frac{l}{L}\right),$$
$$(3)=O\left(A\frac{l}{L}\right),$$
$$(4)=O(A\times 1),$$
$$(5)=O\left[A\left(\frac{l}{L}\right)^{\frac{1}{2}}\right],$$
$$(6)=O\left[A\left(\frac{l}{L}\right)^{\frac{1}{2}}\right],$$
$$(7)=O\left(A\frac{l}{L}\right).$$

Comparing the orders, we see that the most important variable-density term is of the same order as the cross-stream transport. If we discard terms of $O(l/L)^{\frac{1}{2}}$ and higher as $l/L\to 0$ we obtain the crudest sort of local equilibrium assumption, and all terms in density fluctuation are discarded:

$$\langle v^{2}\rangle\frac{\partial U}{\partial y}=\ldots$$
$$=\frac{1}{\langle\rho\rangle}\langle p(u_{,2}+v_{,1})\rangle-\nu\langle u_{,k}v_{,k}\rangle. \tag{4.13}$$

In a similar way, we obtain for the equation for $\langle u^{2}\rangle$:

$$\langle uv\rangle\frac{\partial U}{\partial y}=\frac{1}{\langle\rho\rangle}\langle pu_{,1}\rangle-\nu\langle u_{,k}u_{,k}\rangle, \tag{4.14}$$

for $\langle v^{2}\rangle$:

$$0=\frac{1}{\langle\rho\rangle}\langle pv_{,2}\rangle-\nu\langle v_{,k}v_{,k}\rangle, \tag{4.15}$$

for $\langle uf\rangle$:

$$\langle vf\rangle\frac{\partial U}{\partial y}+\langle uv\rangle\frac{\partial F}{\partial y}=\langle pf_{,1}\rangle, \tag{4.16}$$

for $\langle vf\rangle$:

$$\langle v^{2}\rangle\frac{\partial F}{\partial y}=\langle pf_{,2}\rangle. \tag{4.17}$$

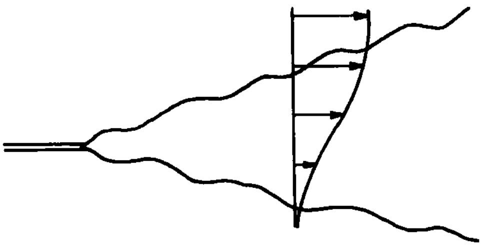

FIGURE 1. Configuration of the constant-density mixing layer.

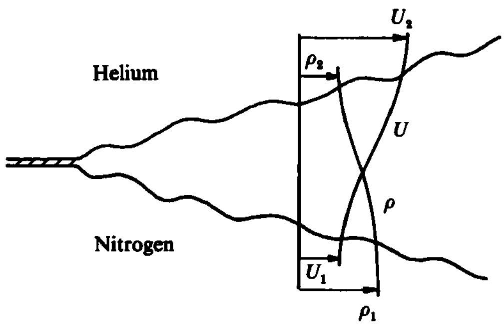

FIGURE 2. Configuration of the helium–nitrogen mixing layer.

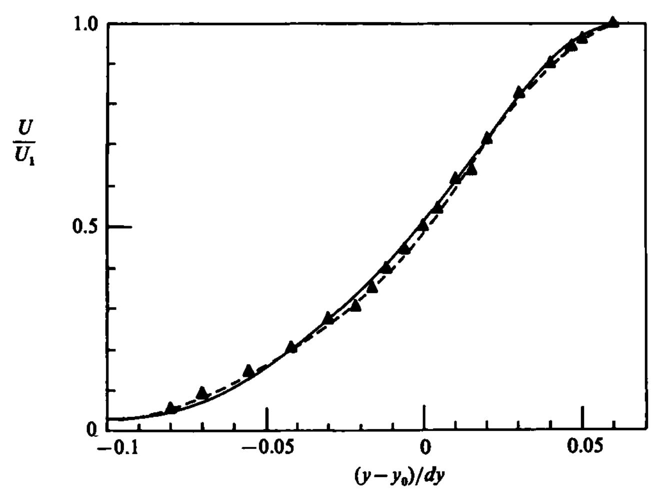

FIGURE 3. Mean velocity in the constant-density mixing layer: ----, simplified equation; ——, full equation; ▲, experiment (Bradshaw *et al.* 1964).

Equations (4.13)–(4.17) are the simplified Reynolds-stress equations and scalar-flux equations, and they are now algebraic equations. We may consider them as an algebraic equation model for Reynolds stress and scalar flux. Note that, even with our worst-case assumption (that is, the 'correction' terms for density are as large as other terms in the equations), taking into consideration our reasoning on the pressure terms, we are reduced to constant-density local equilibrium equations. That is, the turbulence is, to this order, a constant-density turbulence, unaware of the density

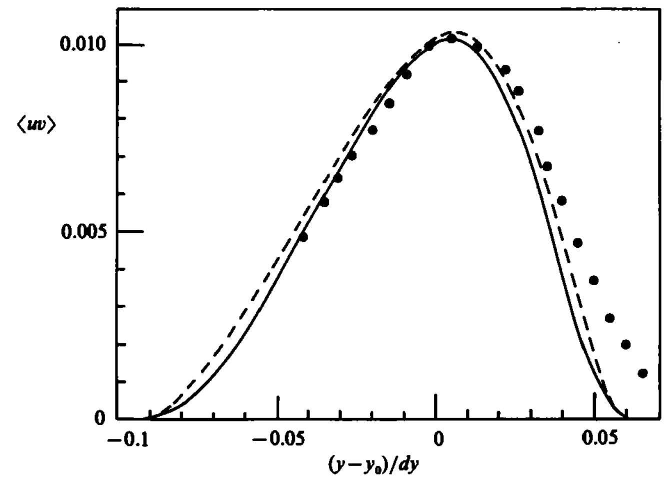

FIGURE 4. Reynolds stress in the constant-density mixing layer: ----, simplified equation; ——, full equation; ●, experiment (Bradshaw *et al.* 1964).

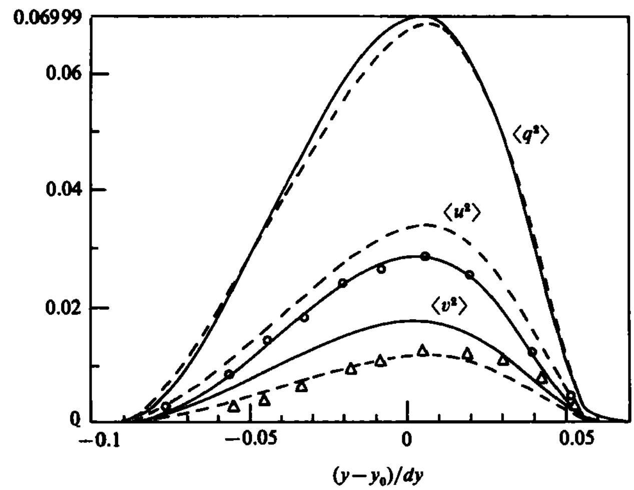

FIGURE 5. Turbulent-energy components in the constant-density mixing layer: ----, simplified equation; ——, full equation; ○, △, experiment (Bradshaw *et al.* 1964).

fluctuations. The non-uniform density makes itself felt only through the continuity and mean-momentum equations. The density fluctuations are produced from the mean-density distribution like fluctuations in a passive scalar. Note that this drastic simplification of the physics would not work in combustion, where there is a physically distinct source of density fluctuations. Using this algebraic-equation model we solve the equations for U, F, $\langle f^2\rangle$, q^2, ϵ_f and ϵ (that is (2.19), (2.20), (2.21), (2.24) and (2.25)).

From a physical point of view, the reason for this surprising result is the following: The most important way in which density fluctuations contribute to the Reynolds-stress equations is through the density fluctuation produced passively from the cross-stream mean-density gradient by the transverse fluctuating velocity. The parcel of fluid carrying this density anomaly makes a contribution to the fluctuations

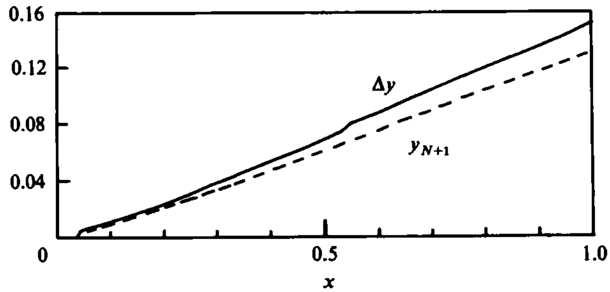

FIGURE 6. Width of the constant-density mixing layer. Δy: evolution of the lateral distance between positions where the velocity is 90 and 10% of the free-stream velocity. y_{N+1}: evolution of the upper edge of computation domain.

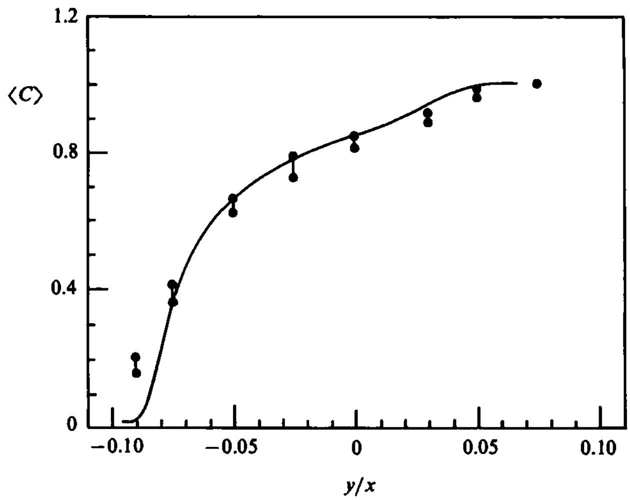

FIGURE 7. Mean mass fraction in the helium–nitrogen mixing layer: ——, simplified equation; ●, experiment (Konrad 1976).

of streamwise or cross-stream momentum proportional to the *product* of the density fluctuation and the velocity fluctuation. This is of second order, and of the same order as the cross-stream transport.

To the extent that the turbulence budget can be regarded as local (dominated by production, dissipation and redistributions among the components) it can also be regarded as uninfluenced by density fluctuations, since these appear only because of transport across the gradient.

5. Results

We have solved both the full equations and the simplified equations for the mixing layer in constant-density and variable-density flows. The full forms of these equations, the models used, the initial conditions and the numerical method can be found in Shih, Lumley & Janika (1985). The experimental data for the constant-density mixing layer were taken from Bradshaw, Ferriss & Johnson (1964) which is considered to contain the best data (Rodi 1972). For the helium–nitrogen mixing layer, the data were provided by Rebollo (1973) and Konrad (1976). Konrad's data

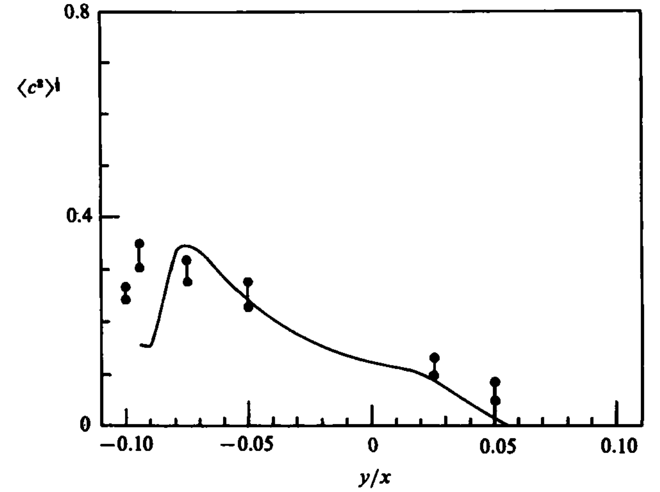

FIGURE 8. Variance of mass-fraction fluctuation in helium–nitrogen mixing layer: ——, simplified equation; ●, experiment (Konrad 1976).

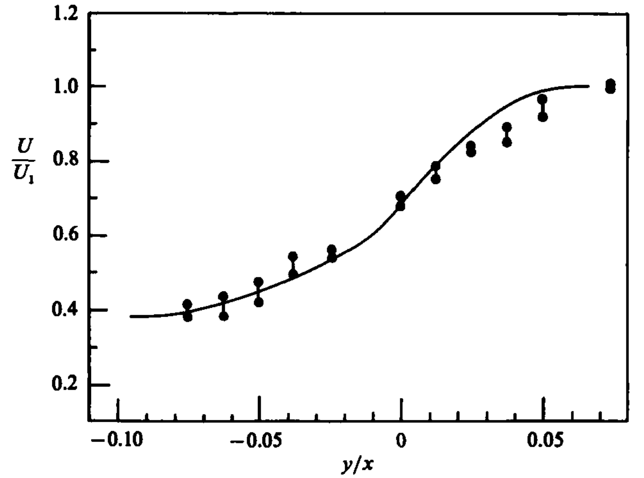

FIGURE 9. Mean velocity in the helium–nitrogen mixing layer: ——, simplified equation; ●, experiment (Konrad 1976).

are considered to be better than those of Rebollo. In our calculation, the mean pressure is constant. Other parameters are:

helium: $\rho = 0.641\ \mathrm{kg/m^3}$, $U = 10.9\ \mathrm{m/s}$,

nitrogen: $\rho = 4.49\ \mathrm{kg/m^3}$, $U = 4.12\ \mathrm{m/s}$.

Figures 1 and 2 are flow configurations for the mixing layers. Figures 3, 4 and 5 are the mean velocity, Reynolds stress and turbulent-energy components for the constant-density mixing layer. The dashed lines and solid lines are solutions for the simplified equations and the full equations respectively. These figures show that our calculations are in good agreement with experiment. If we define a spreading rate as $\mathrm{d}\Delta y/\mathrm{d}x$, Δy being the lateral distance between positions where the velocity is 90

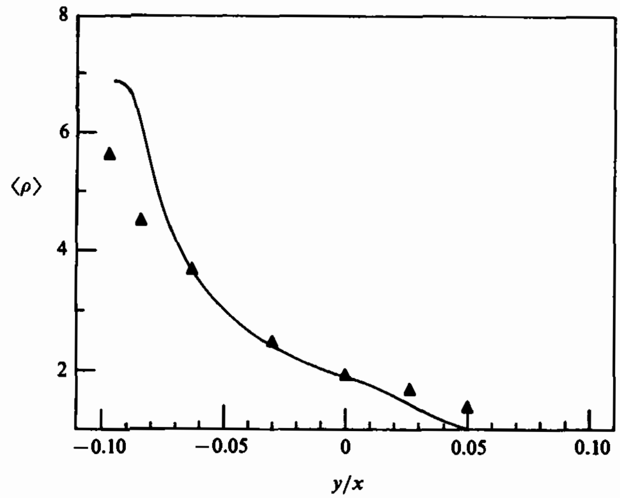

FIGURE 10. Mean density in the helium–nitrogen mixing layer; ——, simplified equation; ▲, experiment (Rebollo 1973).

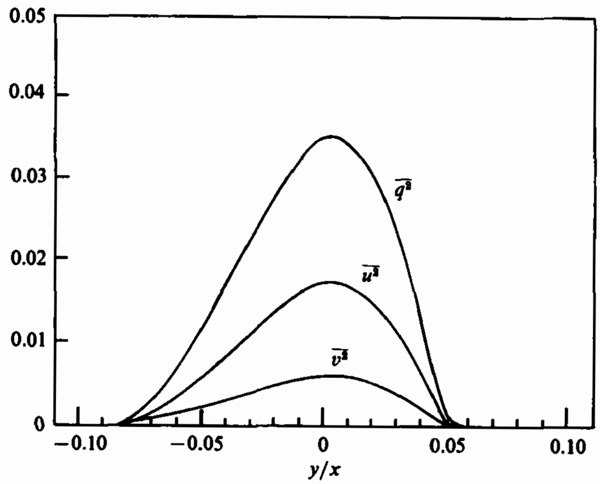

FIGURE 11. Turbulent-energy components in the helium–nitrogen mixing layer: ——, simplified equation.

and 10% of the free-stream velocity (Launder *et al.* 1975), our calculations give a spreading rate of 0.16 (figure 6), which is the same value as Launder's prediction (Launder *et al.* 1975) and quite close to the measurements. Figures 7–12 are the calculations from the simplified equations for the variable-density mixing layer, which show that the solutions do approach self-preservation (we printed out the calculations at $x = 1$ m, 2 m, 3.5 m and 5 m). The experiments mainly provide data on mean mass fraction, variance of mass-fraction fluctuations, mean velocity and mean density. These are shown in figures 7–10. We see that our calculations do reproduce the behaviour of the helium–nitrogen mixing layer. The calculations agree quite well with experiments in the middle part of mixing layer. However, at both edges of the mixing layer, the calculations approach the free-stream values faster than

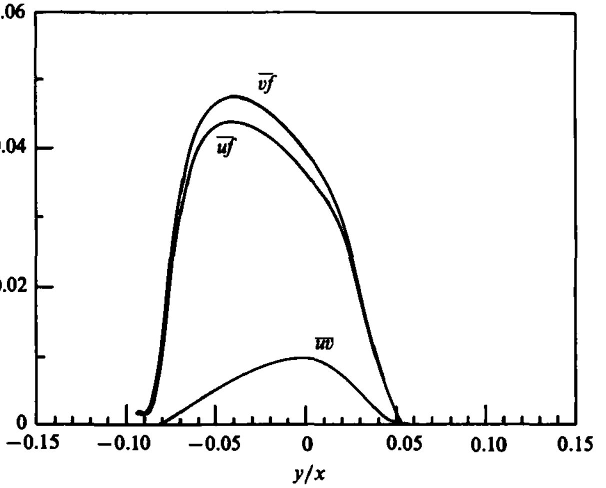

FIGURE 12. Stress and flux in the helium–nitrogen mixing layer: ——, simplified equation.

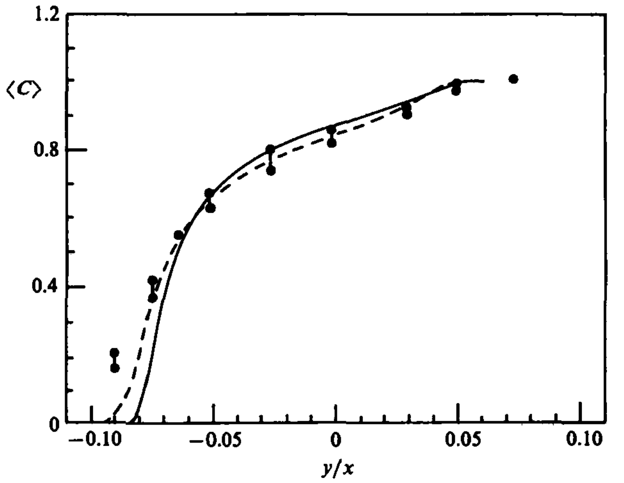

FIGURE 13. Comparison between simplified and full equations (mean mass fraction): ----, simplified equation; ——, full equation; ●, experiment (Konrad 1976).

the experiments. This may suggest that intermittency in variable-density flows is more important than in constant-density flows. Note that in figures 5 and 6, the definition of mass fraction $\langle C\rangle$ is different from F. The relations between $\langle C\rangle$ and F, $\langle c^2\rangle$ and $\langle f^2\rangle$ are as follows:

$$\langle C\rangle = \frac{1+r}{r}\left[1-\frac{1}{rF+1}\right], \tag{5.1}$$

$$\langle c^2\rangle^{\frac{1}{2}} = (1+r)\left[\frac{1}{rF+1}\right]^2 \langle f^2\rangle^{\frac{1}{2}}, \tag{5.2}$$

where $r = (\rho_2-\rho_1)/\rho_1$ and ρ_1, ρ_2 are the densities of nitrogen and helium respectively. Figures 13–15 are the comparisons of the solutions of the full equations and the simplified equations. We see that there is relatively little difference between the two.

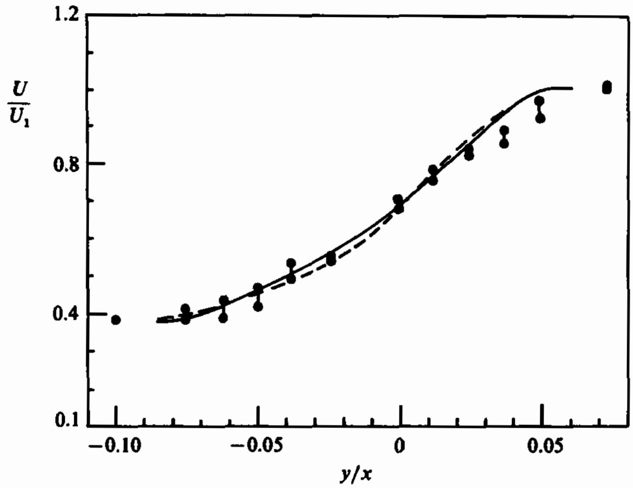

FIGURE 14. Comparison between simplified and full equations (mean velocity): ----, simplified equation; ——, full equation; ●, experiment (Konrad 1976).

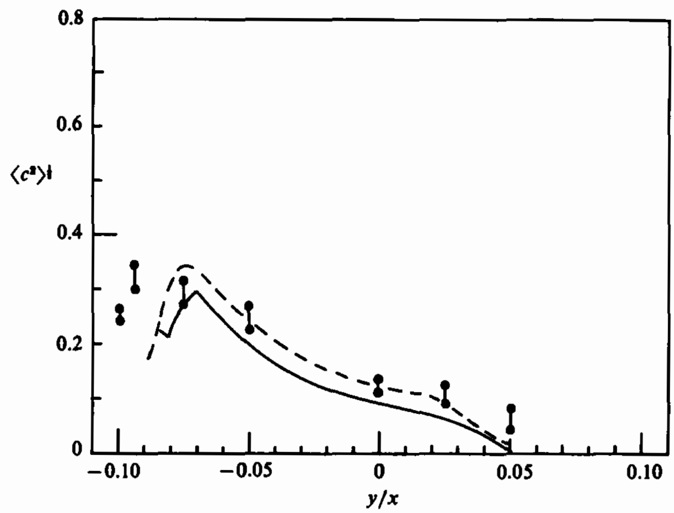

FIGURE 15. Comparison between simplified and full equations (invariance of mass-fraction fluctuations): ----, simplified equation; ——, full equation; ●, experiment (Konrad 1976).

Evidently the simplified equations are quite adequate in thin shear flows. That is certainly a computational convenience since these simplified equations are much easier and faster to solve than the full equations, and the relative lack of cross-coupling makes exploration of new models easier.

However, the fact that the simplified model works so well has taught us something of much greater potential value. We have learned that to a relatively crude local equilibrium approximation, the turbulence is unaffected by density fluctuations; that the density non-uniformity influences only the mean momentum and continuity equations, and is mixed passively down its gradient by the turbulence. This is a sort of Boussinesq approximation for this kind of turbulence which will make the ultimate construction of a model for combustion much easier.

We have also learned that at least in these flows, conventional averaging is more than adequate, and that the modelling can be done as in constant-density flows.

Finally, note that the asymmetry of the mean-density distribution as measured is well reproduced by these models, indicating that the entrainment of low-density and high-density fluid is not symmetric. It has been repeatedly stated that simple models of this type are not capable of reproducing this asymmetry; however, this is evidently not the case. It is also current folk wisdom that it is not possible to model a flow of this type, in which coherent structures are known to play a very significant role, with a model which does not take explicit account of them. This is evidently also not true. The point is that a model of this sort does not know what sort of motions are transporting properties; if the motions, coherent or incoherent, all scale in the same way, it lumps them together.

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