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The influence of buoyancy on turbulent transport

By JOHN L. LUMLEY,† OTTO ZEMAN‡
The Pennyslvania State University, University Park

AND J. SIESS
Établissement Principal, Service Hydrographique et Océanographique de la Marine, Brest, France

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Turbulent transport of fluctuating turbulent energy, turbulent momentum flux, temperature variance, turbulent heat flux, etc. in the upper part of the atmospheric boundary layer is usually dominated by buoyant transport. This transport is responsible for the erosion of the overlying stably stratified region, resulting in progressive thickening of the mixed layer. It is easy to show that a classical gradient transport model for the transport will not work, because it transports energy in the wrong direction. On the other hand, application of the eddy-damped quasi-Gaussian approximation to the equations for the third moments results in a transport model which predicts realistic inversion rise rates and heat-flux profiles. This is also a gradient transport model, but like molecular transport in solutions, a flux of one quantity depends on gradients of all relevant quantities. Transport coefficients are modified by the heat flux, so that the vertical transport is severely reduced near the inversion base. A simple Lagrangian model of transport of an indelible scalar in a stratified flow indicates that the form of the modified transport coefficients results from a marked anisotropic change in the Lagrangian time scale in stratification.

1. Introduction

In an atmospheric boundary layer both buoyancy and wind shear are usually important, but not in the same place. The wind shear is more intense near the surface and falls off strongly with height, while the buoyant forces decrease only slowly with height. If we consider, in particular, a situation typical of early daytime, with both wind and radiant surface heating, producing a surface mixed layer eroding progressively a capping inversion, the wind shear will dominate in the lowest part, where the buoyancy can be neglected, while the wind shear may be neglected in the upper two-thirds (Lumley & Panofsky 1964, p. 74). Again, in the inversion base the abrupt fall-off in vertical transport will usually produce a sharp local wind shear. In the majority of the mixed layer, however, it is buoyancy which is responsible for transporting the variances and fluxes of temperature and momentum to the upper part of the mixed layer, and for the erosion of the inversion, which results in the rise of the inversion base.

Figure 1 (*a*) shows the vertical distribution of vertical variance and turbulent energy

† Present address: Cornell University, Ithaca, New York 14853.

‡ Present address: NOAA Wave Propagation Laboratory, Boulder, Colorado 80309.

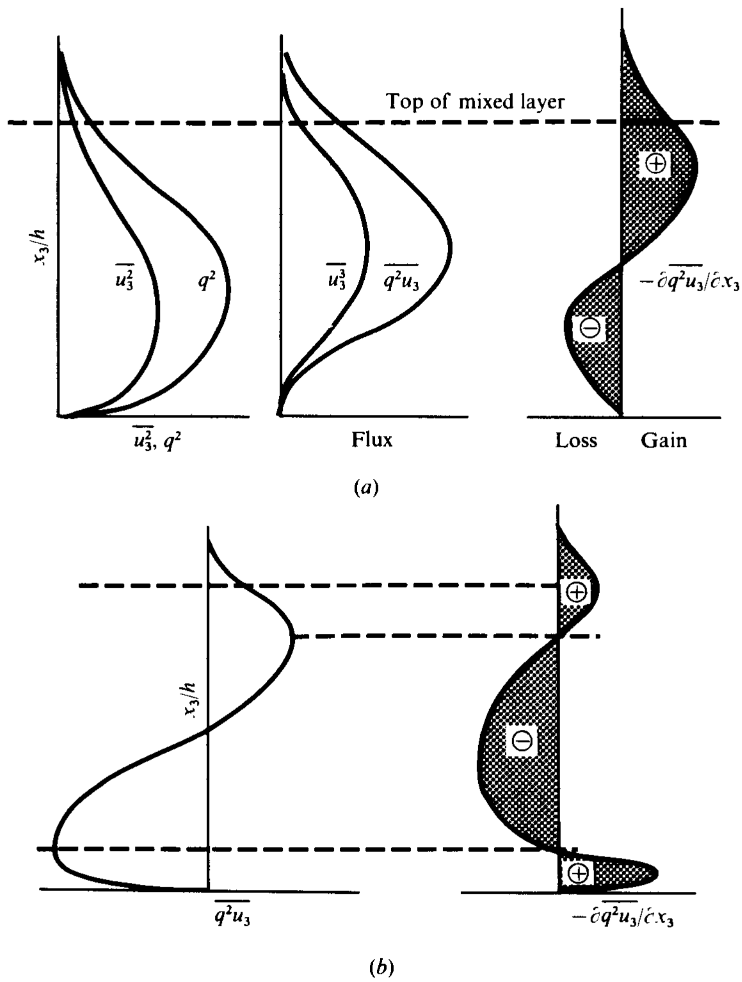

FIGURE 1. (a) Observed profiles of turbulence quantities in buoyancy-driven mixed layers (Zeman 1975). (b) The flux $\overline{q^2u_3}$ and $-\partial(\overline{q^2u_3})/\partial x_3$ as calculated by a scalar transport model (Zeman 1975).

in a convectively driven atmospheric mixed layer, together with the vertical fluxes of vertical variance and energy and the divergence of the flux of turbulent energy (from Zeman 1975). The vertical turbulent transport of turbulent energy must remove turbulent energy from the region near the surface and transport it to the vicinity of the inversion base. In figure 1 (b) we see the form of the divergence of turbulent energy flux which would be produced by a gradient transport model. Energy is now removed from the centre of the layer, and only a fraction is sent up to the inversion base, the remainder being sent down to the surface. Thus a layer powered by a gradient transport model cannot behave properly, and in fact the rise of the inversion base is very poorly predicted, while the vertical distribution of turbulent energy is wildly in error.

The failure of a gradient transport model is, of course, not surprising. The reasons why gradient transport models are not appropriate for turbulence have been extensively discussed (Tennekes & Lumley 1972, pp. 42–50; Corrsin 1974). Summarizing, gradient transport models assume that the length and time scales of the turbulence are small relative to the length and time scales of the mean motion; that is to say, that there is a spectral gap (Lumley & Panofsky 1964, p. 43). This, of course, is rarely the case in a turbulent flow, where the length and time scales of the turbulent motion are usually of the same order as the length and time scales of the mean motion. Nevertheless, there are situations where gradient transport ideas should work; these are situations in which there is locally only one length and time scale in the flow, so that the flux must be proportional to the gradient (and to anything else which has the same dimensions). Since we do not expect that a buoyancy-driven mixed layer will have this simple property, we should not expect a gradient transport model to work.

Nevertheless, in what follows we shall present a technique for constructing a more sophisticated gradient transport model, which does work. We may consider that gradient transport ideas are an outcome of a kinetic-theory approach to turbulence. In a buoyancy-driven mixed layer we have a number of quantities which must be transported (the variances and fluxes); these would play the role of different species in a kinetic-theory approach. We know that molecular transport in salt water, for example, involves a heat flux proportional not only to a temperature gradient, but to a salinity gradient as well (the Dufour effect), while the salt flux is proportional not only to the salinity gradient, but also to the temperature gradient (the Soret effect; Bird, Curtiss & Hirschfelder 1955). If the variances and fluxes in the turbulent situation play the role of species, we may expect that the fluxes of these quantities will involve gradients of all of them. Indeed, a combination of functional and dimensional analysis and invariance theory suggests this (Lumley & Khajeh-Nouri 1974). We shall find, in addition, that there are specific modifications to the transport coefficients by buoyancy.

2. The eddy-damped quasi-Gaussian approximation

Although Lumley & Khajeh-Nouri (1974) suggest a number of different terms which may be present in buoyant transport situations, they all appear with unknown coefficients, and existing experiments are not adequate to determine all their values unambiguously. We need a simple, consistent physical model to do this. Hanjalić & Launder (1972) have suggested a procedure which produces workable equations in the non-buoyant case. They take the equations for the third-order quantities (fluxes of variances and fluxes), neglect convective derivatives, dissipative terms and terms dependent on the mean velocity gradients (all of which can be shown to be about an order of magnitude smaller than the terms retained), replace the fourth-order products which appear explicitly by their quasi-Gaussian form (Monin & Yaglom 1971, p. 233), but replace the pressure correlations, which are integrals over fourth-order products, by relaxation terms, i.e. the third-order term divided by a time scale. Although Hanjalić & Launder do not refer to it by name, the last procedure is essentially the eddy-damped quasi-Gaussian approximation discussed by Orszag (1970). In discussing the failure of the classical quasi-Gaussian approximation, he points out that there is insufficient damping owing to nonlinear interactions and that the spectral transfer produced by the application of the quasi-Gaussian approximation everywhere is reversible, and results in oscillatory behaviour. Representing the pressure integral by an irreversible damping term removes this behaviour. Although the discussion in Orszag (1970) relates to Fourier space, it is equally applicable to real space.

Recently André *et al.* (1976*a*, *b*) have presented another method for dealing with buoyant transport situations. In this approach the quasi-Gaussian approximation is also used for the fourth-order products which appear explicitly, but the pressure correlations are neglected (as are the viscous terms). The resulting equations for the third-order quantities are solved as functions of time. Inequalities for the third-order quantities are derived from Schwarz's inequality, and these inequalities are applied at each time step, the third-order quantities being clipped when they exceed the bounds given by the inequalities. The results obtained from this method, when applied to buoyant convection, are excellent, though not superior to those we shall present. It seems clear, however, that the neglect of the pressure terms permits the third-order quantities to grow too rapidly, and the clipping necessary to prevent their exceeding physically possible values is unphysically abrupt. The fact that excellent results are nevertheless obtained suggests that the results are more dependent on whether certain global conditions are met (in this case realizability), rather than on the details of how those conditions are met. Certainly there are other examples of this sort of insensitivity: the success of the eddy-viscosity approach to turbulence is probably attributable to the fact that the correct amount of momentum is transported in a conservative manner, even though the details of the momentum transport mechanism are not correct.

Although there appears to be no proof that the eddy-damped quasi-Gaussian approximation as used by Hanjalić & Launder (1972) or as used here (in an inhomogeneous situation, with inclusion of the rapid part of the pressure correlations, etc.) satisfies realizability (i.e. assures that the third-order quantities never exceed physically possible values), the fact that Hanjalić & Launder (1972) obtained results in which unphysical behaviour is absent and, in particular, the excellent agreement of our results and those of André *et al.* (1976*a*, *b*) suggest that this is so in some sense. Of the two ways of achieving realizability, we prefer the eddy-damped quasi-Gaussian because (i) it avoids the physically unrealistic clipping, (ii) it can be motivated by various physical arguments and (iii) it leads to equations which can be given a persuasive physical interpretation. In what follows, we shall apply the eddy-damped quasi-Gaussian method to buoyant transport.

For simplicity, let us agree to consider a mixed layer driven entirely by buoyancy, with no mean velocity. We anticipate that the terms in the mean velocity would in any case be negligible (reasoning by analogy with the case of Hanjalić & Launder 1972). Our turbulence will be axisymmetric in the vertical. Let us consider first the equation for $\overline{\theta^2 u_i}$, where θ is the fluctuation in potential temperature and Θ its mean value and we use only the Boussinesq approximation (Lumley & Panofsky 1964, p. 59):

$$\begin{aligned}\dot{\overline{\theta^2 u_i}} = &-(\overline{\theta^2 u_i u_j})_{,j} + \overline{\theta^2}(\overline{u_i u_j})_{,j} + 2\overline{\theta u_i}(\overline{\theta u_j})_{,j} \qquad \mathrm{I}\\ &- 2\Theta_{,j}\overline{\theta u_i u_j} + \beta_i \overline{\theta^3}\\ &- \overline{p_{,i}\theta^2}/\rho \qquad \mathrm{III}\\ &+ \nu\overline{\theta^2 u_{i,jj}} + 2\gamma\overline{\theta u_i \theta_{,jj}}. \qquad \mathrm{II} \qquad (1)\end{aligned}$$

Note that here and throughout we use $(\dot{\;})$ to denote $\partial(\;)/\partial t$ and $(\;)_{,j}$ to denote $\partial(\;)/\partial x_j$; γ is the thermometric diffusivity and β_i is the buoyancy vector, which is directed vertically upwards in the atmosphere and is of magnitude g/T_0, where g is the acceleration due to gravity and T_0 is the adiabatic temperature. By the use of the quasi-Gaussian hypothesis applied to the energy-containing eddies, the group of terms labelled I may be reduced to

$$\mathrm{I} = -\overline{\theta^2_{,j}}\,\overline{u_i u_j} - 2(\overline{\theta u_i})_{,j}\,\overline{\theta u_j}. \tag{2}$$

The quasi-Gaussian hypothesis has been shown by the work of Frenkiel & Klebanoff (1967*a*, *b*) to be justified in homogeneous turbulence. The existence of non-zero third moments, of course, is evidence of a non-Gaussian distribution; the justification for the use of a quasi-Gaussian hypothesis must lie in a perturbation expansion about the Gaussian equilibrium state similar to that of Herring (1965). We shall find that the relaxation time for the third moments is about 20 % of the relaxation time for the second moments; if the relaxation time for each successive cumulant were correspondingly shorter, this would justify using a zero-fourth-cumulant approximation in the equation for the third cumulant, if the overall departure from equilibrium were small.

The molecular transport term, labelled II, may be reduced in the following way (we shall assume for simplicity that $\gamma = \nu$; the case of $\gamma \neq \nu$ can be handled in the same way with slightly greater complexity):

$$\mathrm{II} = \nu(\overline{\theta^2 u_i})_{,jj} - 2\nu(\overline{\theta_{,j}\theta_{,j}u_i}) - 4\nu(\overline{\theta_{,j}\theta u_{i,j}}). \tag{3}$$

In the second term, $\theta_{,j}$ has a spectrum which peaks at wavenumbers in the dissipation range, while u_i has a spectrum which peaks at wavenumbers in the energy-containing range. There is less and less overlap between these ranges as the Reynolds/Péclet number increases, so that the correlation between $\theta_{,j}$ and u_i will go progressively to zero; i.e. the high wavenumber ripples in $\theta_{,j}$ will average out over an excursion of u_i. The quantity $\theta_{,j}\theta_{,j}$, however, is the square of the amplitude of $\theta_{,j}$; if the high wavenumber ripples in $\theta_{,j}$ are modulated by u_i, so that their amplitude increases during an excursion of u_i, then there will be a non-zero correlation regardless of the Reynolds/Péclet number.

The first term is non-zero only because of inhomogeneity, and hence depends on the length scale of this inhomogeneity, which is usually the same as the integral scale in developed turbulence; the ratio of the first and second terms is R_l^{-1}, where R_l is the Reynolds number based on the fluctuating velocity and the integral scale of the turbulence.

The third term can be evaluated by applying the same ideas as were used for the second. Both $\theta_{,j}$ and $u_{i,j}$ have spectra which peak in the dissipative range of wavenumbers, and hence are not well correlated with θ, which has a spectrum which peaks in the energy-containing range. It is possible, however, that if the amplitudes of $\theta_{,j}$ and $u_{i,j}$ are modulated by θ then the combination $\theta_{,j}u_{i,j}$ will have some non-zero contribution, even though it is not a non-negative quantity. We can see, however, that this is not so in the following way: any quantity having its energy at high wavenumbers will not be well correlated with a quantity having its energy at low wavenumbers,† so that we may safely introduce a partial average over the high wavenumber components only. Hence we may consider $\theta_{,j}u_{i,j}$ averaged over the small scales. Now, this is a first-rank tensor, and all isotropic first-rank tensors vanish. The small scales are anisotropic

† θ and $\theta_{,jj}$ appear to be exceptions, since their product $\theta\theta_{,jj}$ can be rewritten as $(\theta\theta_{,j})_{,j} - \theta_{,j}\theta_{,j}$; in a homogeneous flow the average has the value $-\bar{\epsilon}_\theta/\nu$. The correlation *coefficient*, how ever, behaves as $R_l^{-\frac{1}{4}}$.

owing only to the straining of the large scales, and this induced anisotropy decreases as the Reynolds/Péclet number increases. Thus we may expect this small-scale-averaged local quantity to be less and less dependent on the anisotropy of the large scales, and closer and closer to zero, as the Reynolds/Péclet number increases, something which was not true for $\theta_{,j}\theta_{,j}$, which is non-zero even when isotropic. Thus the third term will go to zero as the Reynolds/Péclet number increases.

Hence we are left finally with

$$\mathrm{II} = -2\overline{\epsilon_\theta u_i}, \tag{4}$$

where $\epsilon_\theta = \gamma\theta_{,j}\theta_{,j}$. Hanjalić & Launder (1972) presumed incorrectly that the viscous contribution would vanish at infinite Reynolds/Péclet number: however, it may be neglected in some cases, as we shall see later.

The pressure term III may be separated (following Chou 1945) into a 'rapid' part and a 'return-to-isotropy' part (see also Lumley 1975). That is, we may take the divergence of the instantaneous equation for the velocity, which gives

$$u_{i,j}u_{j,i} = -\nabla^2 p/\rho + \beta_i \theta_{,i}$$

by use of the incompressibility condition. We may define two pressures:

$$0 = -\nabla^2 p^{(1)}/\rho + \beta_i \theta_{,i}$$

and

$$u_{i,j}u_{j,i} = -\nabla^2 p^{(2)}/\rho,$$

where $p = p^{(1)} + p^{(2)}$. We refer to $p^{(1)}$ as the 'rapid' part, because it corresponds in principle to the pressure appearing in rapid-distortion theory (Batchelor & Proudman 1954); i.e. to the neglect of the nonlinear term. Here, of course, it is necessary to generalize rapid distortions to include rapid application of a gravitational field (see Gence 1977). The second term $p^{(2)}$ we refer to as the 'return-to-isotropy' part, because it contains the effect of the nonlinear mixing of the turbulence by itself, which tends to make the turbulence more isotropic (Lumley & Newman 1977). This division is somewhat artificial, of course, since the rapid part also tends to return the turbulence to isotropy under some circumstances.

Taking Fourier transforms, for a homogeneous field we find

$$-\overline{p^{(1)}_{,l}\theta^2}/\rho = -\beta_i \int \overline{\hat\theta\widehat{\theta^2}^*}(\kappa_i\kappa_l/\kappa^2)\, d\boldsymbol{\kappa} \tag{5}$$

for the rapid part; $\hat\theta$ and $\widehat{\theta^2}$ are respectively the Fourier transforms of θ and θ^2, and the asterisk indicates the complex conjugate. The integral is over the entire wavenumber space, and $\boldsymbol{\kappa}$ is the wavenumber vector. We want the simplest possible expression for this part. Since we are considering a near-equilibrium situation, almost homogeneous and almost isotropic, to correspond to the almost-Gaussian assumption, it is natural to take the isotropic value of this term. If we write

$$G_{il} = \int \hat\theta\widehat{\theta^2}^*(\kappa_i\kappa_l/\kappa^2)\, d\boldsymbol{\kappa} \tag{6}$$

we have $G_{il} = G_{li}$ and $G_{ii} = \overline{\theta^3}$. If G_{il} were isotropic, we should have $G_{il} = \frac{1}{3}\overline{\theta^3}\delta_{il}$, for

$$-\overline{p^{(1)}_{,i}\theta^2}/\rho = -\tfrac{1}{3}\beta_i\overline{\theta^3} \tag{7}$$

for the rapid part. For the return-to-isotropy part we shall take

$$-\overline{p^{(2)}_{,i}\theta^2}/\rho = -\overline{\theta^2 u_i}/\mathscr{T}_3, \tag{8}$$

where $\mathscr{T}_3$ is a time scale proportional to $q^2/\bar{\epsilon}$, $\bar{\epsilon}$ being the rate of dissipation of $\frac{1}{2}\overline{q^2}$, where $\overline{q^2} = \overline{u_i u_i}$. Zeman (1975) finds the factor of proportionality in $\mathscr{T}_3$ to be about 0·1. This compares favourably with the value of 0·07 used by Hanjalić & Launder (1972) in the mechanical case, when consideration is taken of their neglect of pressure transport. Equation (8) is the eddy-damping assumption, introducing an irreversible relaxation of $\overline{\theta^2 u_i}$, where $\mathscr{T}_3$ is the relaxation time.

The smallness of the coefficient of proportionality between $\mathscr{T}_3$ and $\overline{q^2}/\bar{\epsilon}$ permits the neglect of (4). That is, if we presume that θ^2 and ϵ_θ are well correlated, which we should expect from the analysis of small-scale intermittency (see, for example, Monin & Yaglom 1975, p. 584), then we can write

$$\overline{\epsilon_\theta u_i} \cong \overline{\theta^2 u_i}\, \overline{\epsilon_\theta}/\overline{\theta^2}. \tag{9}$$

Crude physical reasoning suggests that $\overline{\epsilon_\theta}/\overline{\theta^2} \propto \bar{\epsilon}/\overline{q^2}$ with a coefficient of order unity (see Tennekes & Lumley 1972, p. 95); i.e. that the rate of transfer of $\overline{\theta^2}$ stuff across the θ spectrum is determined by mixing by the energy-containing eddies. A more careful examination of the ratio of these time scales will appear in Newman, Launder & Lumley (1977) and Warhaft & Lumley (1977). For our purposes, however, we need know only that the coefficient is of order unity; then (9) is of the same form as (8), but nearly an order of magnitude smaller.

If we agree to consider slowly changing situations, so that the time derivative may also be neglected (again relative to the relaxation term, so that the slowness of the change need not be too great), we have

$$\overline{\theta^2}_{,j}\, \overline{u_i u_j} + 2(\overline{\theta u_i})_{,j}\, \overline{\theta u_j} = -\overline{\theta^2 u_i}/\mathscr{T}_3 + \tfrac{1}{3}\overline{\theta^3} 2\beta_i - 2\Theta_{,j}\, \overline{\theta u_i u_j}. \tag{10}$$

In exactly the same way, the equation for $\overline{\theta^3}$ may be reduced to

$$\Theta_{,j}\, \overline{\theta^2 u_j} + \overline{\theta^2}_{,j}\, \overline{\theta u_j} = -2\overline{\theta^3}\,\overline{\epsilon_\theta}/\overline{\theta^2}. \tag{11}$$

Here the molecular transport term may not be neglected, since there is no pressure term with which to compare it. If this is substituted in (10), we obtain

$$\begin{aligned} \overline{\theta^2}_{,j}(\overline{u_i u_j} + \beta_i\, \overline{\theta u_j}\, \overline{\theta^2}/3\overline{\epsilon_\theta}) + 2(\overline{\theta u_i})_{,j}\, \overline{\theta u_j} \\ = -\overline{\theta^2 u_i}/\mathscr{T}_3 - \Theta_{,j}\, \overline{\theta^2 u_j}\, \beta_i\, \overline{\theta^2}/3\overline{\epsilon_\theta} - 2\Theta_{,j}\, \overline{\theta u_i u_j}. \end{aligned} \tag{12}$$

Two things are evident: (i) the development of a corrected transport coefficient for $\overline{\theta^2}_{,j}$, which we shall find to occur everywhere when we have obtained equations for all the third-order quantities, and which we shall discuss at that time; (ii) the development of a reduced time scale for vertical transport in the inversion. If the mean temperature gradient is vertical, we shall have an (inverse) relaxation time for vertical transport

$$1/\mathscr{T}_3 + N^2\overline{\theta^2}/3\overline{\epsilon_\theta}, \tag{13}$$

where N is the Brunt–Väisälä frequency. N^2 is positive, of course, in an inversion (corresponding to stability), so that the time scale for vertical transport is correspondingly reduced, relative to that for horizontal transport.

Equation (12) contains another transport term, $\overline{\theta u_i u_j}$, and we must write down the equation for it. The same principles may be applied, the only complication arising with regard to the rapid part of the pressure correlation:

$$(\overline{p_{,i}^{(1)}\theta u_k}+\overline{p_{,k}^{(1)}\theta u_i})/\rho = -\beta_l \int [\widehat{\overline{\theta\theta u_k^*}}(\kappa_i\kappa_l/\kappa^2)+\widehat{\overline{\theta\theta u_i^*}}(\kappa_l\kappa_k/\kappa^2)]\,d\boldsymbol{\kappa}. \quad (14)$$

If we designate the first half of the integral by G_{lik}, then we have $G_{lik}G_{ilk} =$ and $G_{llk} = \overline{\theta^2 u_k}$. In addition, if the field is homogeneous we have $G_{kik} = 0$. This may be obtained from $(\overline{\theta^2 u_k})_{,k} = 0 = 2\overline{\theta\theta_{,k}u_k}$, which implies $\kappa_k \widehat{\overline{\theta\theta u_k^*}} = 0$. If we now assume that G_{lik} may be expressed as a linear combination of the vectors $\overline{\theta^2 u_i}$, we obtain

$$G_{lik} = \tfrac{2}{5}\delta_{li}\overline{\theta^2 u_k} - \tfrac{1}{10}(\delta_{lk}\overline{\theta^2 u_i}+\delta_{ik}\overline{\theta^2 u_l}), \quad (15)$$

so that the equation for $\overline{\theta u_i u_j}$ becomes

$$\Theta_{,j}\overline{u_i u_j u_k}+(\overline{\theta u_i})_{,j}\overline{u_j u_k}+(\overline{\theta u_k})_{,j}\overline{u_j u_i}+(\overline{u_i u_k})_{,j}\overline{\theta u_j}$$
$$= -\overline{\theta u_i u_k}/\mathscr{T}_3+\tfrac{1}{5}\delta_{ik}\beta_l\overline{\theta^2 u_l}+\tfrac{7}{10}(\beta_k\overline{\theta^2 u_i})+\beta_i\overline{\theta^2 u_k})-2\delta_{ik}\bar{\epsilon}\overline{q^2\theta}/3\overline{q^2}. \quad (16)$$

Some of the viscous terms may be neglected relative to the relaxation term, but some may not. Note that we are using the same relaxation time $\mathscr{T}_3$, i.e. assuming that all third-order quantities relax at the same rate. We now have another term appearing, $\overline{u_i u_j u_k}$, and we must write down an equation for this. Again, we obtain an integral representation for the rapid part of the pressure correlation, and assume that it may be represented as a linear function of $\overline{\theta u_k u_l}$, applying the various symmetry and incompressibility requirements, but we find one requirement too few to determine all the coefficients. It is necessary to introduce an appealing, but difficult to justify, assumption to make the form determinate. Specifically, if we define

$$\left.\begin{aligned} G_{pikl} &= \int \overline{\theta \widehat{u_k} u_l^*}(\kappa_p\kappa_i/\kappa^2)\,d\boldsymbol{\kappa}, \\ H_{pikl} &= \int \overline{\widehat{\theta u_k}\widehat{u_l^*}}(\kappa_p\kappa_i/\kappa^2)\,d\boldsymbol{\kappa}, \end{aligned}\right\} \quad (17)$$

we assume that $G_{pikl} = \tfrac{1}{2}(H_{pikl}+H_{pilk})$. This is convenient because an incompressibility condition can be applied to H_{pikl}, but not to G_{pikl}. We obtain for $\overline{u_i u_j u_k}$

$$(\overline{u_i u_k})_{,p}\overline{u_p u_l}+(\overline{u_i u_l})_{,p}\overline{u_p u_k}+(\overline{u_k u_l})_{,p}\overline{u_p u_i}$$
$$= -\overline{u_i u_k u_l}/\mathscr{T}_3+\tfrac{7}{10}(\beta_i\overline{\theta u_k u_l}+\beta_k\overline{\theta u_i u_l}+\beta_l\overline{\theta u_i u_k})+\tfrac{1}{10}(\delta_{ik}\beta_p\overline{\theta u_p u_l}$$
$$+\delta_{il}\beta_p\overline{\theta u_p u_k}+\delta_{kl}\beta_p\overline{\theta u_p u_i})-2\bar{\epsilon}(\delta_{ik}\overline{q^2 u_l}+\delta_{il}\overline{q^2 u_k}+\delta_{lk}\overline{q^2 u_i})/3\overline{q^2}. \quad (18)$$

There are surely other assumptions as appealing as (17). For example, Zeman (1975) has a very approximate technique for deriving forms for all the buoyant terms in these third-moment equations. In the equation for $\overline{u_3^3}$, our form gives $\tfrac{12}{5}\beta\overline{\theta u_3^2}$ while his gives $\tfrac{13}{5}\beta\overline{\theta u_3^2}$; in the equation for $\overline{u_1^2 u_3}$ ours gives $\tfrac{7}{10}\beta\overline{\theta u_1^2}+\tfrac{1}{10}\beta\overline{\theta u_3^2}$ while his gives $\tfrac{1}{5}\beta\overline{\theta u_3^2}$. In the absence of a definitive assumption that can be justified physically, it is comforting to find that physically reasonable assumptions give results that are not very different from one another, and that the differences do not appear to be very significant, since the results of computations with either of the above forms are quite similar.

Similarly, some of the viscous terms can be neglected, and some cannot.

This set of equations (12), (16) and (18) is now closed, and can in principle be solved for the third-order fluxes. For the particular case of a vertically axisymmetric buoyancy-driven mixed layer, we may write the equations in matrix form:

$$-\begin{pmatrix} 1/\mathscr{T}_3+\beta\Theta'\overline{\theta^2}/3\overline{\epsilon_\theta} & +2\Theta' & 0 & 0 & 0 \\ -\frac{8}{5}\beta & 1/\mathscr{T}_3 & 4\bar{\epsilon}/3\overline{q^2} & \Theta' & 0 \\ -\frac{1}{5}\beta & 2\bar{\epsilon}/3\overline{q^2} & 1/\mathscr{T}_3 & 0 & \Theta' \\ 0 & -\frac{12}{5}\beta & 0 & 1/\mathscr{T}_3 & 4\bar{\epsilon}/\overline{q^2} \\ 0 & -\frac{1}{10}\beta & -\frac{7}{10}\beta & 2\bar{\epsilon}/3\overline{q^2} & 1/\mathscr{T}_3 \end{pmatrix}\begin{pmatrix} \overline{\theta^2 w} \\ \overline{\theta w^2} \\ \overline{\theta u^2} \\ \overline{w^3} \\ \overline{u^2 w} \end{pmatrix}$$

$$= \begin{pmatrix} (\overline{\theta^2})'(\overline{w^2}+\beta\overline{\theta w}\overline{\theta^2}/3\overline{\epsilon_\theta})+2(\overline{\theta w})'\overline{\theta w} \\ 2(\overline{\theta w})'\overline{w^2}+(\overline{w^2})'\overline{\theta w} \\ (\overline{u^2})'\overline{\theta w} \\ 3(\overline{w^2})'\overline{w^2} \\ (\overline{u^2})'\overline{w^2} \end{pmatrix}, \tag{19}$$

where a prime denotes $\partial/\partial z$ and the obviously negligible contributions from the viscous terms (those added to the diagonal elements) have been neglected.

The exact inversion of this matrix requires only stamina. An approximate inversion, however, will serve our purpose as well. We make two approximations: first, we presume that the remaining molecular transport terms are negligible, which is justifiable if the various components of the third-order fluxes are of approximately equal size; second, we presume that the influence of gravity (embodied in a suitably non-dimensionalized β) is weak, and we keep only terms of first order in β. We obtain

$$\begin{pmatrix} \overline{w^3} \\ \overline{u^2 w} \\ \overline{\theta w^2} \\ \overline{\theta^2 w} \end{pmatrix}$$

$$= -\begin{pmatrix} 3\mathscr{T}_3 E\left(\overline{w^2}+\overline{\theta w}\dfrac{4}{5E}\beta\mathscr{T}_3\right) & 0 & \frac{24}{5}\beta\mathscr{T}_3^2\overline{w^2} & 0 \\ -\dfrac{3\beta\mathscr{T}_3^3\Theta'}{10}\left(\overline{w^2}-\dfrac{\overline{\theta w}}{3\mathscr{T}_3\Theta'}\right) & \mathscr{D} & \beta\mathscr{T}_3^2\dfrac{\overline{w^2}}{5} & 0 \\ -C\Theta'\mathscr{T}_3^2 3\left(\overline{w^2}-\dfrac{\overline{\theta w}}{3\mathscr{T}_3\Theta'}\right) & 0 & 2\mathscr{T}_3 C\left(\overline{w^2}+\dfrac{8}{5}\dfrac{\beta\mathscr{T}_3}{C}\overline{\theta w}\right) & \overline{w^2}\frac{8}{5}\mathscr{T}_3^2 \\ 6\mathscr{T}_3^3\Theta'^2 B\left(\overline{w^2}-\dfrac{\overline{\theta w}}{3\mathscr{T}_3\Theta'}\right) & 0 & -4\mathscr{T}_3^2\Theta' B\left(\overline{w^2}-\dfrac{\overline{\theta w}A}{2\mathscr{T}_3\Theta' B}\right) & \mathscr{F} \end{pmatrix}$$

$$\times\begin{pmatrix} (\overline{w^2})' \\ (\overline{u^2})' \\ (\overline{\theta w})' \\ (\overline{\theta^2})' \end{pmatrix}, \tag{20}$$

where
$$A = 1-\beta\mathscr{T}_3^2\Theta'\left(\frac{\theta^2}{3\bar{\epsilon}_\theta\mathscr{T}_3}+\frac{16}{5}\right),\qquad \mathscr{D} = \mathscr{T}_3 D\left(\overline{w^2}+\overline{\theta w}\frac{7}{10}\frac{\beta\mathscr{T}_3}{D}\right),$$
$$B = 1-\beta\mathscr{T}_3^2\Theta'\left(\frac{\overline{\theta^2}}{3\bar{\epsilon}_\theta\mathscr{T}_3}+\frac{28}{5}\right),$$
$$C = 1-\tfrac{28}{5}\beta\mathscr{T}_3^2\Theta',$$
$$D = 1-\tfrac{7}{10}\beta\mathscr{T}_3^2\Theta',\qquad \mathscr{F} = \mathscr{F}_3 A\left(\overline{w^2}+\frac{\beta}{A}\frac{\overline{\theta^2}}{3\bar{\epsilon}_\theta}\overline{\theta w}\right).$$
$$E = 1-\tfrac{12}{5}\beta\mathscr{T}_3^2\Theta',$$

Zeman (1975) has generated a complete inversion, as well as an even more approximate one; (20) is somewhere between the two in accuracy. The various multipliers $A, \ldots, E$ have clearly been reduced to the form $1-aN^2\mathscr{T}_3^2$ by the assumption that the influence of β is small; they should all be replaced in computations by $(1+aN^2\mathscr{T}_3^2)^{-1}$. Note that $\overline{\theta u^2}$ is not necessary in the computation.

3. Interpretation of the buoyant transport

The diagonal terms in (20) are of exactly the form resulting from the Priestley–Swinbank effect (1947) extensively discussed by Deardorff (1966, 1972), and produce a counter-gradient vertical heat flux. To see this, consider a homogeneous buoyant flow without mean velocity in an approximately steady state and modelled according to Donaldson (1972; see also Lumley 1975):

$$\Theta_{,i}\overline{\theta u_i} = -\bar{\epsilon}_\theta, \tag{21a}$$
$$\Theta_{,j}\overline{u_i u_j} = -\overline{\theta u_i}/\mathscr{T}_2+\tfrac{2}{3}\beta_i\overline{\theta^2}. \tag{21b}$$

Defining
$$\mathscr{T}_\theta = c\overline{\theta^2}/\bar{\epsilon}_\theta, \tag{22}$$
(21 a) becomes
$$\overline{\theta^2} = -\mathscr{T}_\theta\Theta_{,i}\overline{\theta u_i}/c, \tag{23}$$
which may be inserted in (21 b) to give
$$\overline{\theta u_i} = -\mathscr{T}_2\{\overline{u_j u_i}+\overline{\theta u_j}\beta_i\mathscr{T}_\theta(2/3c)\}\Theta_{,j}. \tag{24}$$
In fact, in this artificially homogeneous situation the heat flux cannot be against the gradient [from (23)]; a flux divergence is necessary to produce this effect. In a stable situation, however, when the vertical heat flux is negative, the vertical transport will be substantially reduced.

We may construct a simple physical model which will explain the presence of the additional terms in the diagonal diffusion coefficients of (20), or in (24). Consider gradient transport of temperature, presumed indelible. Then we can write in a homogeneous field (without mean velocity)
$$\theta(\mathbf{x},t) = -\Theta_{,i}(x_i-X_i(\mathbf{x},t|0)), \tag{25a}$$
with
$$X_i(\mathbf{x},t|t') = x_i+\int_t^{t'}u_i(\mathbf{X}(\mathbf{x},t|t''),t'')\,dt'',$$

and

$$\overline{\theta u_i} = \Theta_{,j}\,\overline{u_i(\mathbf{x},t)\,(x_j - X_j(\mathbf{x},t|0))},$$

with

$$\overline{u_i(\mathbf{x},t)\,(x_j - X_j(\mathbf{x},t|0))} = \int_0^t \overline{u_i(\mathbf{x},t)\,u_j(\mathbf{X}(\mathbf{x},t|t''),t'')}\,dt'', \tag{25b}$$

where we presume t to be large. $\mathbf{X}(\mathbf{x},t|t')$ is the position at time t' of the material point which is at $\mathbf{x}$ at t. Now, in a flow with buoyancy, a moving parcel of fluid is subject to acceleration due to buoyancy. We can write very approximately $\dot{u}_i = \beta_i\theta$ for the additional acceleration. Thus a hot parcel, for example, will be accelerated upwards until it has penetrated far enough into the gradient to reverse the temperature anomaly (since it is presumed to carry its temperature indelibly) and hence the vertical velocity will be quite persistent. We are accustomed to write in non-buoyant homogeneous flows

$$\int_0^\infty \overline{u_i(\mathbf{x},t)\,u_j(\mathbf{X}(\mathbf{x},t|t''),t'')}\,dt'' = \overline{u_i u_j}\mathscr{T}, \tag{26}$$

which presumes that the Lagrangian integral time scale is the same regardless of direction; this is clearly only an approximation in an anisotropic non-buoyant homogeneous flow, an approximation which is likely to be worse the larger the anisotropy. In a buoyant homogeneous flow it is certainly not true. A point moving upwards will have a much larger integral scale than a point moving horizontally. We can approximate this by considering an artificial velocity field $u_i^0(\mathbf{x},t')$ which at $t' = t$ is identical with $u_i(\mathbf{x},t)$. For $t' > t$, however, $u_i^0(\mathbf{x},t')$ evolves with $g = 0$ (or with uniform temperature, which is equivalent). Then we can write

$$u_i(\mathbf{X}(\mathbf{x},t|t'),t') = u_i^0(\mathbf{X}(\mathbf{x},t|t'),t') + \alpha\int_t^{t'} \beta_i\,\theta(\mathbf{X}(\mathbf{x},t|t''),t'')\,dt'', \tag{27}$$

where α is an unknown coefficient. This is presumably correct only to first order, since there will be a nonlinear contribution from the inertial terms. We may now form the integral in (26):

$$\int_0^t \overline{u_i(\mathbf{x},t)\,u_j(\mathbf{X}(\mathbf{x},t|t'),t')}\,dt'$$
$$= \int_0^t \overline{u_i(\mathbf{x},t)\,u_j^0(\mathbf{X}(\mathbf{x},t|t')}\,dt' + \alpha\beta_j\int_0^t dt'\int_t^{t'} \overline{u_i(\mathbf{x},t)\,\theta(\mathbf{X}(\mathbf{x},t|t''),t'')}\,dt''. \tag{28}$$

Now, the first integral may safely be written as (26), while the second integral may be written as

$$\int_0^t dt'\int_t^{t'} \overline{u_i(\mathbf{x},t)\,\theta(\mathbf{X}(\mathbf{x},t|t''),t'')}\,dt'' = -\overline{u_i\theta}\int_0^t dt'\int_{t'}^t dt''\rho(t''-t)$$
$$= -\overline{u_i\theta}\int_0^t (t-\tau)\,\rho(-\tau)\,d\tau. \tag{29}$$

Now the correlation coefficient $\rho(-\tau)$ will have zero integral, since u_i is stationary and θ is the derivative of a stationary quantity (Tennekes & Lumley 1972, p. 216). This is a necessary condition for the integral in (29) to have a finite limit. We expect the limit to be negative; this can be seen if we make a simple non-mixing model of the motion of the parcel of fluid in a temperature gradient; we obtain

$$\rho(-\tau) = \cos\mu\tau + (\Theta'\overline{w^2}/\mu\overline{\theta w})\sin\mu\tau, \tag{30}$$

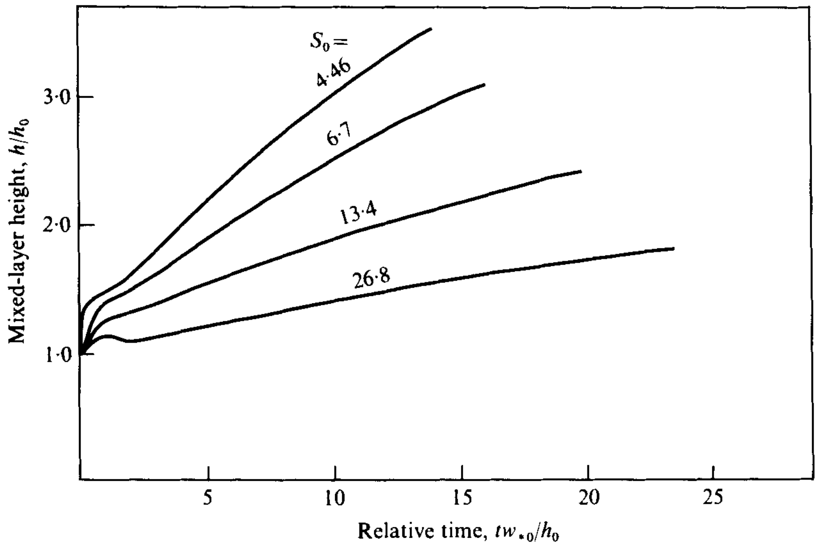

FIGURE 2. Inversion rise rates (Zeman 1975). S_0 is the initial value of the buoyancy parameter $\gamma_i h_0/T_{*0}$, where γ_i is the inversion lapse rate, h_0 is the initial mixed-layer height and T_{*0} is the initial value of the characteristic r.m.s. temperature fluctuations in free convection, given by $\overline{\theta w_0}/w_{*0}$, where $\overline{\theta w_0}$ is the surface heat flux and $w_{*0} = (\beta\overline{\theta w_0}\,h_0)^{\frac{1}{3}}$. Here $h_0 = 200$ m, $w_{*0} = 1$ m/s and $T_{*0} = 0{\cdot}15$ °C.

where $\mu^2 = \Theta'/\beta$ (treating the stable case). The coefficient $\Theta'\overline{w^2}/\mu\overline{\theta w} < 0$ in a homogeneous steady flow. The integral is asymptotically proportional to $\Theta'\overline{w^2}t/\mu^2\overline{\theta w}$ (the limit is not finite here, because the form (30) does not have zero integral, since it is without mixing). Thus we can write

$$-\overline{u_i\theta}\alpha\beta_j\int_0^t (t-\tau)\rho(-\tau)\,d\tau \to \overline{u_i\theta}\alpha\beta_j\mathscr{T}\mathscr{T}_\theta \qquad (31)$$

since the integral has the dimensions of (time)^2 and the coefficient of proportionality has been absorbed in α. Hence we have for the diffusion coefficient

$$\mathscr{T}\{\overline{u_iu_j}+\alpha\beta_j\overline{u_i\theta}\mathscr{T}_\theta\}, \qquad (32)$$

which is essentially the same form as (24).

Note that if $\beta_3 > 0$ and $\overline{w\theta} < 0$, corresponding to an upward flux entering an inversion, there is a considerable reduction in the upward diffusion coefficient

$$\mathscr{T}\{\overline{w^2}+\alpha\beta\mathscr{T}_\theta\overline{w\theta}\}$$

since the entering parcels of fluid have roughly

$$\overline{q^2} = (\mathscr{T}/c)\,\beta\overline{\theta w}|_0 \qquad (33)$$

(from the definition of $\mathscr{T}$, and the fact that the dissipation is roughly the production, which is given almost entirely by $\beta\overline{\theta w}$), where $\overline{\theta w}|_0$ is the value entering the inversion;

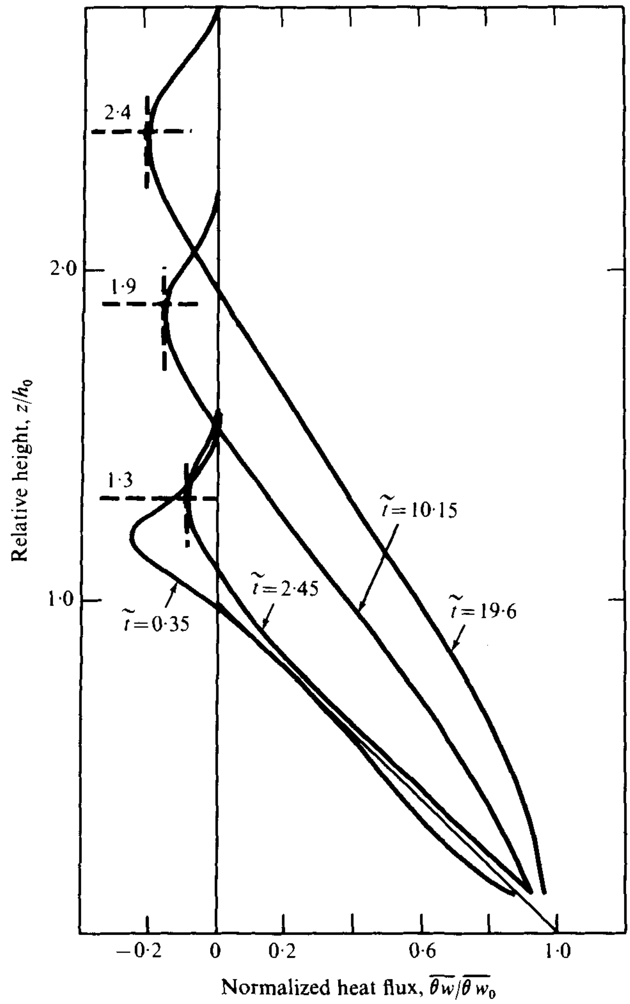

FIGURE 3. Heat-flux profiles (Zeman 1975). S_0 is the initial value of the buoyancy parameter $\gamma_i h_0/T_{*0}$. Here $h_0 = 200$ m, $\overline{\theta w_0} = 0{\cdot}15$ °C m s^{-1}, $S_0 = 13{\cdot}4$ and $\tilde{t} = tw_{*0}/h_0$.

at the top of the mixing region at the inversion base, the entering heat flux is approximately reversed, so that the diffusion coefficient (32) becomes roughly

$$\frac{\mathscr{T}^2}{c}\beta\overline{\theta w}|_0\left(\frac{\overline{w^2}}{\overline{q^2}}-\frac{2}{3}\right) \qquad (34)$$

if we take $\alpha = 2/3c$ and $\mathscr{T}_\theta = \mathscr{T}$. Hence the diffusion coefficient is capable of going to zero at the top of the entrainment layer, as it should.

4. Computational verification and discussion

A computation of this vertically axisymmetric buoyancy-driven flow was carried out using second-order modelling techniques and a simplified version of (20). The details are reported in Zeman (1975).† Realistic inversion rise rates and heat-flux profiles

† The only difference between the results from computing with (20) and with Zeman's (1975) version, which is not linearized in buoyancy (though simplified in other respects), is a (negative) value of the energy flux at the surface (see figure 5) about twice as large.

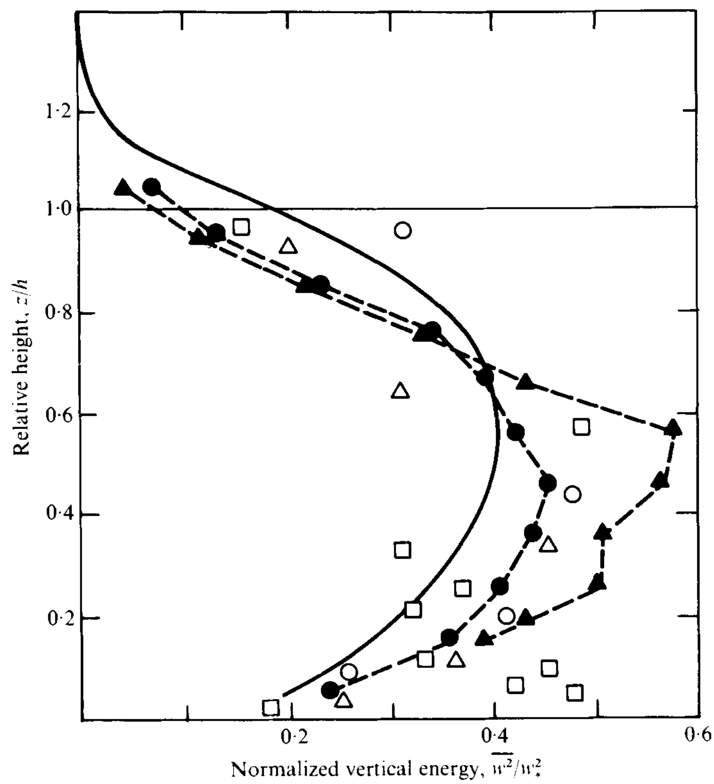

FIGURE 4. Predicted vertical energy compared with experimental data (from Zeman & Lumley 1976). –●–, Willis & Deardorff (1974), case *S1* ($S = 90$); –▲–, Willis & Deardorff (1974), case *S2* ($S = 200$); ○, △, Lenschow (1970, 1974), Lenschow & Johnson (1968); □, Telford & Warner (1964).

(figures 2 and 3) were obtained. Attention should be drawn to the negative region of the heat-flux profiles at the inversion base. This negative region, which corresponds to the overshoot in the mean temperature profile, indicates that the entrainment of stably stratified fluid at the inversion base is being correctly modelled. Since the mixed-layer dynamics in this case are entirely dependent on the model for the third-order fluxes, this is a strong indication that this model is broadly correct.

The material presented in figures 2 and 3 is somewhat indirect. Of greater interest are the fluxes themselves. In figures 4 and 5 respectively we present the vertical energy and flux of turbulent energy compared with measurements (both from Zeman & Lumley 1976). It can be seen that the computed values are qualitatively as sketched in figure 1 (*a*) and compare favourably with measurements.

Note that, although (20) is a gradient transport form, the dependence of each flux on the gradients of several quantities saves it from the errors of the simplistic version presented in figure 1 (*b*). Looking at $\overline{w^3}$ for example, the downward transport in the lower half of the layer resulting from the gradient of $\overline{w^2}$ is more than offset by the transport resulting from the gradient of the heat flux.

In the statistical mechanics of mixtures, there are restrictions on the possible values of the diffusion and cross-diffusion coefficients. Here there are also restrictions,

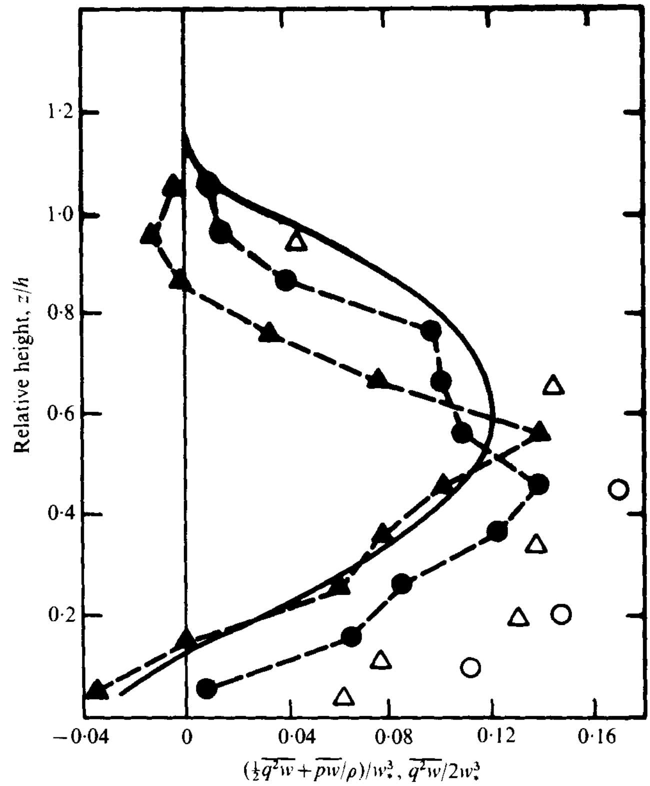

FIGURE 5. Predicted fluxes of turbulent energy compared with data (from Zeman & Lumley 1976). ——, $(\frac{1}{2}\overline{q^2w}+\overline{pw}/\rho)/w_*^3$; other symbols as in figure 4.

corresponding to the requirement that the eigenvalues of the diffusion coefficient matrix in (20) should have non-negative real parts. This is essentially the same restriction as for molecular transport; there, however, the second law of thermodynamics is responsible, requiring that gradients should not become more steep. In the turbulent case, stability considerations produce the same requirement. If the real part of any of the eigenvalues of the matrix in (20) were negative, small ripples in the distribution of any of the second-order quantities would be amplified indefinitely. From a computational point of view, it is thus essential that some restriction be placed on the values of the coefficients in (20). There does not appear to be any convenient necessary and sufficient condition that will guarantee that all eigenvalues will have positive real parts. Schumann (1976) has recently shown that a necessary, though not sufficient, condition is that all diagonal coefficients K_{ii} (no sum) be positive and that

$$K_{ji}K_{ij} < K_{ii}K_{jj},$$

$i \neq j$ (no sum). A necessary and sufficient condition would be that all determinants of all orders that can be formed which are symmetric about the diagonal be positive; of course, many of these conditions would be redundant, since the classical condition is that the uppermost determinant of each order symmetric about the diagonal be positive (Jeffreys & Jeffreys 1956, p. 137).

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