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Turbulence Modelling in Naturally Convecting Fluids

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ABSTRACT

In this report an introduction to turbulence modelling is presented, with applications to heat transfer in a molten pool. The turbulence closure problem is discussed and some approximations and methods are given for determining certain unknowns in the transport equations. Three methods of closure are given. These are: the $k - \epsilon$ model; the algebraic-stress model and the full Reynolds Stress model, this last being the most general of the three. Finally, we apply two of these closures to the problem of a strongly convective flow. We show that these provide a turbulent solution in the limit of steady-state and no mean flow. However, it is an open question as to whether the physics of a strongly convective flow can be realistically modelled by such closures.

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1. Introduction.

For many years, researchers in fluid mechanics have been interested in the regime of high Reynolds number, in which it has been known since the time of O. Reynolds (1883) that the flow becomes turbulent at high velocities (or equivalently, low viscosity). In many fluid flow problems, particularly in engineering applications, one often only encounters turbulence which is generated by shear in the flow, in which the important quantity is the gradient of the mean velocity field. However, in the study of the safety of nuclear fission reactors, one is often more concerned with buoyancy-driven flows and in this case, it is the Rayleigh number Ra, defined in equation (1.1) below, which is the important quantity.

$$Ra = \frac{\beta\, g\, \Delta T\, L^3}{\alpha\, \nu}. \tag{1.1}$$

Where,

β is the coefficient of thermal expansion,
g is the gravitational acceleration,
$\Delta T = T - T_\infty$ is a temperature difference across the fluid,
L is a length scale,
α is the thermal diffusivity
and ν is the coefficient of kinematic viscosity.

The Rayleigh number is a dimensionless quantity which expresses the ratio of convective to diffusive transport of energy.

In a fission reactor, one is concerned with the highly unlikely possibility that a nuclear core may suffer prolonged loss of cooling. In this scenario a significant fraction of the core may melt, leading to the formation of a molten pool within the reactor pressure vessel. It is therefore of interest to study the natural convection heat transfer within such pools, with the aim of predicting the heat flux to surrounding structures or coolant. The Rayleigh numbers for these events are expected to be of the order of $Ra = 10^{11} - 10^{12}$, and the flow is almost certain to be strongly turbulent at such high Rayleigh numbers. In the past investigators have modelled heat transfer from the flow based on the representation of the heat transfer coefficient by a Nusselt number, Nu. In turn, the Nusselt number is calculated by the use of correlations of the form,

$$Nu = CRa^{\gamma}, \tag{1.2}$$

where C and γ are constants to be determined by fits to the experimental data. These correlations are extrapolated from the scarce experimental data which are generally given for Rayleigh numbers many orders of magnitude less than those required and often for a much simplified geometry (cf. Turland and Morgan, 1985).

Faster computers and more efficient codes, however, should allow one to model the heat transfer directly from the Navier-Stokes equations, probably with the addition of equations describing the turbulence. However, there are problems associated with this approach. When a fluid is strongly convecting (large Ra) and is contained within rigid walls, then the mean flow will be restricted to a narrow boundary layer around the walls (Wild, 1983). Outside this layer, the fluid is expected to be essentially stagnant, with the only motion being provided by small, convective cells of turbulent fluid having a random distribution of velocities. In a scenario of this type, one would expect the mean flow to be approximately zero everywhere except within the boundary layer. (There is an assumption here that the flow is fully turbulent, so that the mean flow really can be distinguished from the turbulent quantities.) Difficulties arise because existing turbulence models are constructed in such a way that a non-zero mean flow is assumed. Nevertheless, a study to determine if the codes presently available are able to model the molten pools better than current heat-transfer correlations is being undertaken by the author. To this end, it has been necessary to review the current state of turbulence modelling and this is the purpose of this paper. Throughout this report, we are concerned only with the study of natural convection. We assume that the term "convection" is synonymous with "natural convection", although of course this is not true in general.

In section 2, we derive the turbulent transport equations from the Navier-Stokes equation and discuss the turbulence closure problem. In section 3, we look at methods of closure and in section 4 we use these to study the problem of buoyancy driven turbulence. Finally, we present the conclusions in section 5.

2. Conservation Equations in Turbulent Flow.

A turbulent flow is generally assumed to be one in which the physical quantities describing the flow vary in an irregular, non-repeatable way. The flow is then assumed to be chaotic, but with a character which must still obey the basic conservation equations of classical fluid mechanics. In describing a turbulent flow, one begins with the equation of continuity, the Navier-Stokes equation, and one or more equations describing the scalar fields (i.e. changes in chemical composition, heat transfer etc.). The physics of the flow is then contained within the solutions to these equations, together with the appropriate boundary conditions, and in general these solutions will comprise the variables velocity $\tilde{V}_i$, pressure $\tilde{P}$, density $\tilde{\rho}$, temperature $\tilde{\Theta}$ and chemical concentration $\tilde{\Xi}$, where a tilde indicates that the variable may exhibit turbulence.

In what follows, we will impose the assumptions of an incompressible fluid and an isotropic concentration of one chemical species. We can thus replace the turbulent density $\tilde{\rho}$ by a constant density ρ and the equation in $\tilde{\Xi}$ decouples from our set of equations. (These assumptions are reasonable, since in our application we are dealing with liquid UO_2, and for the present no other material is involved.)

Noting that we sum over repeated suffixes, the equations describing the flow are:

$$\frac{\partial \tilde{V}_i}{\partial x_i} = 0 \qquad (2.1)$$

$$\frac{\partial \tilde{V}_i}{\partial t} + \tilde{V}_j \frac{\partial \tilde{V}_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \tilde{P}}{\partial x_i} + \frac{1}{\rho}\frac{\partial}{\partial x_j}\left(\mu \frac{\partial \tilde{V}_i}{\partial x_j}\right) + \tilde{F}_i / \rho \qquad (2.2)$$

$$\frac{\partial \tilde{\Theta}}{\partial t} + \tilde{V}_j \frac{\partial \tilde{\Theta}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \tilde{\Theta}}{\partial x_j}\right) + \tilde{S}_\Theta / \rho c. \qquad (2.3)$$

Here, the independent variables are the co-ordinate vector x_i and time t. We have assumed a constant specific heat capacity c, and the fluid viscosity and thermal diffusivity are denoted by μ and Γ respectively. $\tilde{F}_i$ is the body force and $\tilde{S}_\Theta$ is a volumetric heating term.

In order to model the turbulence it is convenient to think of it as consisting of a (random) fluctuation superimposed upon a mean quantity. Furthermore, the fluctuations are considered to be only local and since they are assumed random, we would physically expect their time average to be zero, if one integrates over a sufficiently long time. Thus, if one writes, for the velocity, say,

$$\tilde{V}_i = V_i + v_i, \tag{2.4}$$

where v_i is the fluctuation in velocity, then the mean velocity V_i is formally defined as,

$$V_i(t_0) = \frac{1}{T} \int_{t_0 - T/2}^{t_0 + T/2} \tilde{V}_i \, dt. \tag{2.5}$$

This last equation is valid for both stationary and non-stationary mean flows, providing that over some characteristic averaging time T, the change in V_i is small. Thus, the mean quantity may still be a function of time providing the time-scale of change is very much greater than T. If this is not the case, then the time average defined above would not be a useful variable in studying the turbulence, and one must resort to some other method. In this report, however, it is assumed that formulae such as (2.5) above will always be valid.

One may also define the mean of other physical variables, and in general, the average of a variable $\tilde{\Phi}$ is defined as,

$$\Phi(t_0) = \frac{1}{T} \int_{t_0 - T/2}^{t_0 + T/2} \tilde{\Phi} \, dt, \tag{2.6}$$

and we can always write

$$\tilde{\Phi} = \Phi + \phi. \tag{2.7}$$

From now on, we will always denote fluctuations by a lower case character and the time average mean defined above by the upper case equivalent. At this point, we should also note that the taking of a derivative with respect to a spatial variable commutes with the averaging process. That is, we may write,

$$\overline{\frac{\partial \phi'}{\partial x_i}} = \frac{\partial \overline{\phi'}}{\partial x_i}, \tag{2.8}$$

where ϕ' represents a product of fluctuations, so that the average is non-zero.

Returning to equations (2.1) to (2.3), we may replace each quantity with a tilde above it by the relevant fluctuation plus mean. Furthermore, we remember that, by definition, the time averages of fluctuations are zero and that the average of a mean is just the mean. We may average equations (2.1) to (2.3), denote an averaged quantity by an overbar (if the quantity is not a mean) and write:

$$\frac{\partial V_i}{\partial x_i} = 0 \tag{2.9}$$

$$\frac{\partial V_i}{\partial t} + V_j \frac{\partial V_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \frac{1}{\rho}\frac{\partial}{\partial x_j}\left(\mu \frac{\partial V_i}{\partial x_j} - \rho\overline{v_i v_j}\right) + F_i/\rho \tag{2.10}$$

$$\frac{\partial \Theta}{\partial t} + V_j \frac{\partial \Theta}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \Theta}{\partial x_j} - \overline{v_j \theta}\right) + S_\Theta/\rho c. \tag{2.11}$$

Equation (2.9) above is just the continuity equation for an incompressible fluid. Equations (2.10) and (2.11), on the other hand, are identical to the Navier-Stokes and heat transfer equations respectively, except that they contain additional transport terms due to the turbulent fluctuations. In the first of these equations, momentum (per unit volume) is transferred from one point to another by the gradient of the so-called Reynolds stresses, $\overline{v_i v_j}$, whilst in the latter, it is the heat which is transported by the turbulent scalar heat flux $\overline{v_i \theta}$. Note that this quantity is really a vector and the name is merely conventional.

These equations form a set of five simultaneous partial differential equations. However, the variables number fourteen (in three dimensions and assuming that the quantities F_i and S_Θ can be written in terms of the other variables) and are: the six components of the Reynolds stress (the Reynolds stress tensor is symmetric), three components of the scalar heat flux, three components of the mean velocity, the pressure and the temperature. In order to completely specify and solve the problem, one must either derive further equations in the unknown elements, or somehow approximate them in what would hopefully be a physical way. The latter of these is the most practical route, since, as we shall now see, the derivation of further equations in the (unknown) turbulent quantities leads to the origin of further unknowns, and the set of equations is again not closed. This problem has long troubled turbulence modellers and is at the root of all lack of progress in turbulent modelling. It is known as the Turbulence Closure Problem.

In order to model the turbulent quantities and hence determine the fluid flow, one would often prefer to work with transport equations in the Reynolds stresses and scalar heat flux in addition to the turbulent equivalent of the Navier-Stokes and heat transfer equations. In this way, one obtains more information regarding the fluctuations and about their transport through the fluid than one would get by, perhaps more naïvely, approximating them by some product of a length scale and a shear, as is done in the so-called zeroth-order closure (see, for example, Bradshaw et. al., 1981). The methods analysed here are thus two-equation models, with a second-moment closure scheme (although we do refer to one equation models for completeness).

To derive our transport equations, we first of all take the Navier-Stokes equation (2.2), multiply by v_k, replace $\tilde{V}_i$ etc by the sum of a fluctuation and a mean, average and add to the result the analogous equation with i and k interchanged. We then obtain the Reynolds stress transport equation (2.12) below:

$$
\begin{aligned}
\frac{\partial \overline{v_i v_k}}{\partial t} + V_j \frac{\partial \overline{v_i v_k}}{\partial x_j} = & \underbrace{-\left(\overline{v_i v_j}\frac{\partial V_k}{\partial x_j} + \overline{v_j v_k}\frac{\partial V_i}{\partial x_j}\right)}_{P_{ik}} \underbrace{+ \left(\overline{f_i v_k} + \overline{f_k v_i}\right)/\rho}_{G_{ik}} \\
& \underbrace{+\overline{\frac{p}{\rho}\left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i}\right)}}_{\Phi_{ik}} \\
& \underbrace{-\frac{\partial}{\partial x_j}\left(\overline{v_i v_j v_k} + \frac{\overline{p v_k}}{\rho}\delta_{ij} + \frac{\overline{p v_i}}{\rho}\delta_{jk} - \nu \frac{\partial \overline{v_i v_k}}{\partial x_j}\right)}_{d_{ik}} \\
& \underbrace{-2\nu \overline{\frac{\partial v_i \, \partial v_k}{\partial x_j \, \partial x_j}}}_{\epsilon_{ik}} . \qquad (2.12)
\end{aligned}
$$

Terms on the left-hand side of (2.12) have been grouped according to convention and in the best way to illustrate physical processes. The terms grouped above P_{ik} represent rates of creation of $\overline{v_i v_k}$ by the mean shear, whilst G_{ik} represents rates of creation by the body force f_i or f_k. The first of these terms needs no approximation in the level of closure which we are considering here, and providing the only body forces present are linear in velocity or temperature, then G_{ik} can also be left in its exact form. (Linear body forces include gravity and rotation. In the former, the Boussinesq approximation is generally imposed in order to represent f_i in terms of θ.)

The d_{ik} represent diffusion, as can be seen by integrating this term over a volume bounded by rigid surfaces. The integral vanishes, indicating that these terms make no contribution to the dissipation or production of the Reynolds stresses, but serve to redistribute the stresses (Leslie, 1973). The terms Φ_{ik} likewise do not contribute to the production of Reynolds stresses, rather they attempt to make the stresses isotropic by removing contributions from the cross terms $\overline{v_i v_j}$. They have no effect on the turbulent kinetic energy, $k = \overline{v_i v_i}\,/\,2$, since the trace of Φ_{ik} is zero, from the equation of continuity. Finally, ϵ_{ik} represents removal of energy by viscous forces, and much of turbulence modelling is based upon determining a reasonable approximation for these terms.

We thus see that again we have encountered the turbulent closure problem, where in deriving a transport equation for the Reynolds stresses, we have produced further unknowns in the form of the terms denoted by Φ_{ij}, d_{ij} and ϵ_{ij}. These terms must be suitably approximated before any further progress can be made in solving these equations. We look at this problem further in section 3.

The transport equation for the scalar flux contains similar terms, and is derived by multiplying equation (2.3) by v_i and adding it to equation (2.2) multiplied by θ. The result is given in equation (2.13), where we have neglected the heating term S_Θ for simplicity. The remaining terms have a similar physical interpretation to the analogous ones appearing in equation (2.12). $P_{i\theta}$ represents the production of the scalar heat flux by the mean velocity and temperature gradients, whilst $G_{i\theta}$ is again the production due to a body force. The quantity $d_{i\theta}$ is clearly diffusive, whilst $\epsilon_{i\theta}$ is taken to be dissipative, since this is the only term which can limit the growth of $\overline{v_i\,\theta}$. Finally, $\Phi_{i\theta}$ is again assumed to redistribute the scalar heat flux evenly among all the elements.

$$
\begin{aligned}
\frac{\partial \overline{v_i\,\theta}}{\partial t} + V_j \frac{\partial \overline{v_i\,\theta}}{\partial x_j} = & \underbrace{-\left(\overline{v_i\,v_j}\frac{\partial \Theta}{\partial x_j} + \overline{v_j\,\theta}\frac{\partial V_i}{\partial x_j}\right)}_{P_{i\theta}} \underbrace{+\overline{f_i\,\theta}/\rho}_{G_{i\theta}} + \underbrace{\overline{\frac{p}{\rho}\frac{\partial \theta}{\partial x_i}}}_{\Phi_{i\theta}} \\
& \underbrace{-\frac{\partial}{\partial x_j}\left(\overline{v_i\,v_j\,\theta} + \frac{\overline{p\,\theta}}{\rho}\,\delta_{ij} - \Gamma\,\overline{v_i\,\frac{\partial \theta}{\partial x_j}} - \nu\,\overline{\theta\,\frac{\partial v_i}{\partial x_j}}\right)}_{d_{i\theta}} \\
& \underbrace{-\left(\Gamma + \nu\right)\overline{\frac{\partial \theta\,\partial v_i}{\partial x_i\,\partial x_j}}}_{\epsilon_{i\theta}}. \qquad (2.13)
\end{aligned}
$$

The unknown terms in equation (2.13) are: $G_{i\theta}$, $\Phi_{i\theta}$, $d_{i\theta}$ and $\epsilon_{i\theta}$. Again, we must make suitable approximations in order to fully specify the problem.

We now have the necessary basic knowledge and equations to allow us to begin a study of turbulence closure, and we will do this in the next section. We should perhaps first mention, however, that in deriving equations (2.12) and (2.13), we have generated the most general turbulence model available at this level of closure, and for many problems, the amount of detail which the solutions provides us with may not be necessary. Often it is sufficient to work with the turbulent kinetic energy, defined by $k = \overline{v_i v_i}/2$, and in section 3 we will consider such models.

3. Turbulence Closure Schemes.

In this section, we look at some of the approximations which enable us to close the turbulence equations of the previous section. Unfortunately, the nature of the turbulence closure problem does not allow a general method of closure, since many schemes rely on experimental results. Therefore, approximations can be made only for specific problems.

Turbulence modelling is made more difficult for strongly convecting flows for two reasons. The first is that very few experiments have been performed for high Rayleigh number flows, and even those results that do exist are often for Rayleigh numbers far below those required for strongly turbulent flow (see section 1). However, Goldstein and Tokuda (1980) attained a Rayleigh number of 10^{11} for water and derived a Nusselt number correlation based on their results. It is difficult to ascertain the relevance of this correlation to the flows under consideration in this report and the reason for this is that, in our application, the boundary conditions must be taken into account when deriving a heat-transfer correlation. Turland and Morgan (1985) and Turland (1989) summarised this problem and noted that different correlations can exist for different boundaries, even though the Rayleigh number is the same. It is for this reason that a more general model must be developed and why we are considering turbulence closure schemes in this report. Reviews of some of the experiments which are relevant to the type of problem we are considering may be found in Turland and Morgan (1985).

The second reason why turbulence modelling is difficult in our application is really a consequence of the first, and is that, for many years, models have been constructed on the basis of shear-driven turbulence, for which there are numerous experimental data available in the literature. Those wishing to study convection-driven turbulence are therefore at a huge disadvantage, since there is no convenient starting point. They either have to invent a whole new set of turbulence closure schemes, which presumably would be based on current, shear-driven turbulence models, or they must apply the current models in the hope that they give "reasonable" results.

Thompson et al. (1985) and Wilkes and Thompson (1986), for example, studied the double-glazing and analogous problems using standard models. They found that there was an incompatibility between these models and results from a boundary layer analysis (George and Capp, 1979). This is perhaps not surprising. On the one hand, boundary layer theory provides one with a solution by asymptotic expansion of the equations describing the convecting fluid, whilst on the other hand, a turbulence model is used which has little relevance to the flow it purports to model. The reason is, as we have stated earlier, that the current turbulence models are based on a shear flow, which is not necessarily the strongest driving force present in these types of flow. Nevertheless, such models may be convenient in studying qualitative properties of the flow, and this is one of the uses to which Thompson et al. and Wilkes and Thompson put them.

In the remainder of this section we will study three representative turbulence closure schemes, noting that they are all based upon shear-generated turbulence. Their relevance to high Rayleigh number flows is not discussed until section 4.

3.1 The $k - \epsilon$ model.

The starting point for this model is the equation for the transport of the Reynolds stresses, equation (2.12) of section 2, with the indices k and i equal. Summing over repeated indices, we obtain an equation in the turbulent kinetic energy per unit mass, defined in three dimensions as

$$k = (\overline{v_1^2 + v_2^2 + v_3^2})/2. \tag{3.1}$$

The transport equation for the turbulent kinetic energy is:

$$\begin{aligned} \frac{\partial k}{\partial t} + V_j \frac{\partial k}{\partial x_j} &= -\overline{v_i v_j}\frac{\partial V_i}{\partial x_j} + \overline{f_i v_i} - \nu \left(\overline{\frac{\partial v_i}{\partial x_j}\frac{\partial v_i}{\partial x_j}} \right) \\ & -\frac{\partial}{\partial x_j}\left(\frac{\overline{v_i v_i v_j}}{2} + \overline{\frac{p}{\rho} v_i}\delta_{ij} - \nu \frac{\partial k}{\partial x_j} \right). \end{aligned} \tag{3.2}$$

The physical meaning of the various terms in this equation correspond to the analogous ones in equation (2.12) of section 2. Note, however, that the pressure-strain terms Φ_{ii} are identically zero due to the equation of continuity (see also section 2). Furthermore, the buoyancy terms are generally neglected and, in this case, an equation in the scalar heat flux $\overline{v_i\,\theta}$ is not required.

In this approximation, the unknown terms which have to be modelled in order to close the equation are the diffusion, the viscous dissipation and the Reynolds stresses, $\overline{v_i\,v_j}$. The first of these consists of two contributions, one due to viscosity, $\nu\,(\partial k\,/\,\partial x_j)$ and one due to turbulent diffusion, $\overline{v_j\,(v_i\,v_i + p\,\delta_{ij}/\rho)}$. In order to estimate the turbulent diffusion term, it is always assumed that it takes the same form as the diffusion due to viscosity, so that

$$\overline{\frac{v_i\,v_i\,v_j}{2} + \frac{p}{\rho}\,v_i\,\delta_{ij}} = -\frac{\nu_t}{\sigma_k}\,\frac{\partial k}{\partial x_j}. \tag{3.3}$$

In equation (3.3), σ_k is a turbulent Prandtl number which is used to fit the model to experimental data and the important concept of the kinematic eddy viscosity ν_t has been introduced. For dimensional reasons, ν_t is taken to be proportional to the product of a velocity scale and a length. If the velocity scale is assumed to be proportional to the square root of the turbulent kinetic energy (Kolmogorov, 1942; Prandtl, 1945), then one can write:

$$\nu_t = c_\mu\,k^{\frac{1}{2}}\,L, \tag{3.4}$$

where c_μ is an empirical constant and L is a length scale assumed to be characteristic of the turbulence and is often called the mixing length (see, for example, Spalding and Launder, 1972). Equation (3.4) is the Kolmogorov-Prandtl relation.

The viscous dissipation is usually replaced by ϵ, where ϵ is defined as

$$\epsilon = \nu\,\overline{\frac{\partial v_i}{\partial x_j}\,\frac{\partial v_i}{\partial x_j}} \tag{3.5}$$

and we must derive a further relation in ϵ so that we have closure. In the one-equation models, one does this by assuming a high Reynolds number flow, so that dissipation is independent of the kinematic viscosity ν. The quantity ϵ is then a function only of k and the characteristic length, L (Launder and Spalding, 1972). Dimensionally, we must have,

$$\epsilon = k^{3/2}/L. \tag{3.6}$$

The reasons for choosing to replace an unknown dissipation ϵ by another unknown L are largely because L is more easily estimated from experiment and from physical reasoning.

Unfortunately, such one-equation models, like the zero-equation model briefly discussed in section 2, do not contain information about changes in the length scale L. For example, dissipation processes can destroy the smaller eddies, thus increasing the relative number of large scale eddies. Also, advection plays a rôle in transporting eddies downstream, so that the length scale at any point is dependent upon the size of eddies upstream.

For this reason two-equation models are to be preferred over one-equation closures. The $k - \epsilon$ two-equation model involves an equation in the transport of turbulent kinetic energy, k and one in the dissipation, ϵ. The Kolmogorov-Prandtl relation is still employed in order to specify the turbulent viscosity, and equation (3.6), relating ϵ to k and L, is used so that the dissipation equation is written in terms of ϵ rather than L. The Kolmogorov-Prandtl relation then becomes:

$$\nu_t = c_\mu k^2 / \epsilon. \tag{3.7}$$

The equation representing the variation of the dissipation is complicated and will not be given here. Readers are referred to Harlow and Nakayama (1968) for more information. Suffice it to say that the equation contains several new correlations which have limited physical interpretation and for which rather drastic approximations have to be made. Hanjalić and Launder (1972) proposed the following approximate form for this equation:

$$\frac{\partial \epsilon}{\partial t} + V_j \frac{\partial \epsilon}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{c_\mu}{\sigma_\epsilon} \frac{k^2}{\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] - c_{1\epsilon} \frac{\epsilon}{k} \overline{v_i v_j} \frac{\partial V_i}{\partial x_j} - c_{2\epsilon} \frac{\epsilon^2}{k}, \quad (3.8)$$

where we have taken into account the molecular viscosity ν. The constants $c_{1\epsilon}$ and $c_{2\epsilon}$ are assumed to be universal constants whose values, together with c_μ and the Prandtl numbers σ_ϵ and σ_k, are determined from experiment. There seems to be good agreement between the values of these quantities (compared in Bradshaw et al., 1981) and, like Rodi (1987), we will take the values of Launder and Spalding (1972).

This formalism is complete only when approximations to the Reynolds stresses have been made. Boussinesq (1877) hypothesized that the Reynolds stresses could be modelled by writing:

$$\overline{v_i v_j} = -\nu_t \frac{\partial V_i}{\partial x_j}. \quad (3.9)$$

A modified form of the original Boussinesq hypothesis appears below and is to be preferred for two reasons. Firstly, the new equation is valid when $i = j$. Secondly, the Reynolds stresses are supposed to be symmetric under an interchange of the indices i and j. However, in the original Boussinesq equation, $\overline{v_i v_j} \neq \overline{v_j v_i}$, and the hypothesis is not valid unless the extra constraint is imposed that the mean shears are isotropic. The more recent approximation does possess this symmetry property under an interchange of indices and is

$$\overline{v_i v_j} = -\nu_t \left(\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} \right) + \frac{2}{3} k \, \delta_{ij}. \quad (3.10)$$

With all these approximations, the $k - \epsilon$ model becomes:

$$\begin{aligned}\frac{\partial k}{\partial t} + V_j \frac{\partial k}{\partial x_j} &= \nu_t \left(\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} \right) \frac{\partial V_i}{\partial x_j} \\ &+ \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{c_\mu}{\sigma_k} \frac{k^2}{\epsilon} \right) \frac{\partial k}{\partial x_j} \right] - \epsilon \end{aligned} \tag{3.11}$$

$$\begin{aligned}\frac{\partial \epsilon}{\partial t} + V_j \frac{\partial \epsilon}{\partial x_j} &= c_{1\epsilon} \frac{\nu_t \epsilon}{k} \left(\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} \right) \frac{\partial V_i}{\partial x_j} \\ &+ \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{c_\mu}{\sigma_\epsilon} \frac{k^2}{\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] - c_{2\epsilon} \frac{\epsilon^2}{k} \end{aligned} \tag{3.12}$$

and these equations (3.11) and (3.12), along with equation (3.7) and equations (2.9) to (2.11) of section 2, form a turbulence closure model.

3.2 Inclusion of Scalar Heat Flux in the $k - \epsilon$ Model.

If one wishes to include the body forces in the above model, then one must make further approximations. If the only body force present is gravity, then the terms $\overline{f_i v_i}$ are usually calculated via the Boussinesq approximation, in which density fluctuations are only taken into account when multiplied by a gravitational acceleration, g_i. Thus, it is assumed that the force fluctuations are due to buoyancy, which in turn is induced by the action of gravity on small, local variations in density. These fluctuations in body force (per unit volume) are then assumed to be given by:

$$f_i = \rho' g_i, \tag{3.13}$$

where, ρ' is the fluctuation in density.

One can replace ρ' by a temperature fluctuation by using the coefficient of thermal expansion, β, which is assumed constant and is defined as

$$\beta = -\frac{1}{\bar{\rho}} \frac{\partial \bar{\rho}}{\partial \bar{\Theta}} \bigg|_{p=\text{constant}.} \tag{3.14}$$

If ρ_0 is the density at the reference temperature Θ_0, then multiplying through by g_i and replacing the derivative by $(\bar{\rho} - \rho_0) / (\bar{\Theta} - \Theta_0)$ gives us:

$$\rho \beta (\Theta + \theta - \Theta_0) g_i = -\rho' g_i \equiv -f_i \tag{3.15}$$

since the "reference" density ρ_0 must be the same as the incompressible density ρ. Multiplying through by v_i and time averaging gives the relationship that we require:

$$\overline{f_i v_i} = -\beta \rho \overline{v_i \theta} g_i. \tag{3.16}$$

In order to model this equation, many authors make an analogy with the Boussinesq hypothesis (see, for example, Launder, 1976), and write

$$\overline{v_i \theta} = -\frac{\nu_t}{\sigma_\theta} \frac{\partial \Theta}{\partial x_i} \tag{3.17}$$

and the equations are again closed.

The equations describing the turbulence are the same as equations (3.11) and (3.12) of the previous sub-section, except for an addition of one term in each. The new equations are:

$$\begin{aligned} \frac{\partial k}{\partial t} + V_j \frac{\partial k}{\partial x_j} &= \nu_t \left(\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} \right) \frac{\partial V_i}{\partial x_j} \\ &+ \beta g_i \frac{\nu_t}{\sigma_\theta} \frac{\partial \Theta}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{c_\mu}{\sigma_k} \frac{k^2}{\epsilon} \right) \frac{\partial k}{\partial x_j} \right] - \epsilon \end{aligned} \tag{3.18}$$

$$\frac{\partial \epsilon}{\partial t} + V_j \frac{\partial \epsilon}{\partial x_j} = c_{1\epsilon} \frac{\nu_t \epsilon}{k} \left(\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} \right) \frac{\partial V_i}{\partial x_j}$$
$$+ c_{1\epsilon} c_{3\epsilon} \frac{\epsilon}{k} \beta g_i \frac{\nu_t}{\sigma_\theta} \frac{\partial \Theta}{\partial x_i}$$
$$+ \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{c_\mu}{\sigma_\epsilon} \frac{k^2}{\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] - c_{2\epsilon} \frac{\epsilon^2}{k}, \qquad (3.19)$$

where $c_{3\epsilon}$ is an extra constant to be determined. The merits of this type of closure for convective flows will be discussed in section 4.

3.3 The Algebraic Stress Model

The algebraic stress model (ASM) can be thought of as a generalisation of the eddy-viscosity model discussed above. The Reynolds stresses are still represented by algebraic formulae, but now, the approximations are more broadly applicable. The model was developed for computational efficiency and the basic idea involves replacing the derivatives in the Reynolds stress and scalar heat flux transport equations (equations (2.12) and (2.13)) with algebraic formulae. In this way, all numerical integrations and the need for a model of the diffusion are avoided.

The starting point of the model is to assume that the time variation and "net diffusion" (that is, advection plus diffusion) of the Reynolds stresses can be expressed in terms of transport of kinetic energy. Rodi (1972, 1976) suggested the following relationship:

$$\frac{\partial \overline{v_i v_j}}{\partial t} + diff(\overline{v_i v_j}) = \frac{\overline{v_i v_j}}{k} \left(\frac{\partial k}{\partial t} + diff(k) \right), \qquad (3.20)$$

where diff indicates the "net diffusion", and is defined by

$$diff(\overline{v_i v_j}) = V_k \frac{\partial \overline{v_i v_j}}{\partial x_k} - d_{ij}$$
$$diff(k) = V_k \frac{\partial k}{\partial x_k} - d_{ii}. \qquad (3.21)$$

Here, d_{ij} and d_{ii} represent the diffusion of $\overline{v_i v_j}$ and k respectively, as expressed in equations (2.12) and (3.2).

Now, the transport of turbulent kinetic energy can be expressed in the following form, according to equation (3.2) and the second of equation (3.21):

$$\frac{\partial k}{\partial t} + \mathit{diff}(k) = P + G - \epsilon, \qquad (3.22)$$

where P and G represent the production of turbulent kinetic energy due to shear and body forces respectively and ϵ is the dissipation. Note that these three quantities do not contain any terms which need to be integrated.

We can substitute equation (3.22) into equation (3.20) in order to model the transport of Reynolds stresses. We obtain:

$$\frac{\partial \overline{v_i v_j}}{\partial t} + \mathit{diff}(\overline{v_i v_j}) = P_{ij} + G_{ij} + \Phi_{ij} + \epsilon_{ij} = \frac{\overline{v_i v_j}}{k}(P + G - \epsilon), \qquad (3.23)$$

the first equality being due to equation (2.12). The analysis is complete if the unknowns Φ_{ij} and ϵ_{ij} can be modelled. These terms have been approximated in Launder (1975) and Gibson and Launder (1978). The resulting quantities, as with the P_{ij} and G_{ij}, do not contain any terms which require integration. We can therefore substitute the approximations for Φ_{ij} and ϵ_{ij} into equation (3.23) and rearrange the last two equalities to obtain an algebraic relationship in the Reynolds stresses. The result is:

$$\overline{v_i v_j} = k \left\{ \frac{2}{3}\delta_{ij} + \frac{(1 - c_2)\left(\frac{P_{ij}}{\epsilon} - \frac{2}{3}\delta_{ij}\frac{P}{\epsilon}\right) + (1 - c_3)\left(\frac{G_{ij}}{\epsilon} - \frac{2}{3}\delta_{ij}\frac{G}{\epsilon}\right)}{c_1 + \frac{P + G}{\epsilon} - 1} \right\}. \qquad (3.24)$$

In a similar way, the scalar heat flux can be modelled by writing

$$\frac{\partial \overline{v_i \theta}}{\partial t} + diff(\overline{v_i \theta}) = \frac{\overline{v_i \theta}}{k}(P + G - \epsilon) \tag{3.25}$$

and the scalar heat fluxes are then given by (Gibson and Launder, 1978; Rodi, 1987):

$$\overline{v_i \theta} = \frac{\frac{k}{\epsilon}\left\{\overline{v_i v_j}\frac{\partial \theta}{\partial x_j} + (1 - c_{2\theta})\left(\overline{v_j \theta}\frac{\partial V_i}{\partial x_j} + \beta g_i \overline{\theta^2}\right)\right\}}{c_{1\theta} + \frac{1}{2}\left(\frac{P+G}{\epsilon} - 1\right)}. \tag{3.26}$$

Note that the algebraic stress model requires the $k - \epsilon$ model in addition to equations (3.24) and (3.26), since the quantities k and ϵ still occur in these algebraic formulae. However, the advantage of this model is that information is obtained regarding transport of the Reynolds stresses and scalar heat flux. In order to close the model, a relation in $\overline{\theta^2}$ is required. However, we will defer an analysis of this quantity until a later section.

3.4 Full Reynolds Stress Closure

This scheme represents the most general model available at this level of closure, and should perhaps be preferred for this reason. The advantage of this closure is that it provides one with the greatest amount of information regarding the transport of the Reynolds stresses and scalar heat flux, something that the $k - \epsilon$ model cannot possibly do. However, there are at least six extra equations to be added to the seven of the $k - \epsilon$ model and the computational time will be greatly increased.

As before, the method involves making approximations to the various unknown terms in the transport equations. In a Reynolds stress closure, these unknowns are ϵ_{ij}, $\epsilon_{i\theta}$, Φ_{ij}, $\Phi_{i\theta}$, d_{ij}, $d_{i\theta}$ and $G_{i\theta}$, according to the discussion in section 2. The contributions from each of these quantities will of course depend upon the properties of the fluid and the geometry of the problem one wishes to study. A general set of approximations cannot be constructed which will model every flow. Therefore, in order to simplify the equations, one often chooses to work in the regime of high Reynolds number flows, and this is what we shall do in the remainder of this report.

Choosing a high Reynolds number flow has two important effects. Firstly, the viscosity becomes less important in the transport of the large-scale turbulence. Secondly, the small-scale turbulence is independent of the structure of the mean flow or any large scale turbulence that may be present. In this limit of high Reynolds number, the small scale turbulence tends towards isotropy. Information regarding direction which the large-scale turbulence possesses on account of the mean velocity field is not passed down to the smaller scales (Bradshaw, 1976; Tennekes and Lumley, 1972).

Unfortunately, these properties have been attributed to turbulence driven by a mean shear and are not necessarily applicable to buoyant flows, although it is not clear why such flows would be non-isotropic in the small scale. However, the mathematical simplification offered by an isotropic flow is an important factor to take into account and, for this reason, we assume that any inaccuracies which the assumption of isotropy may introduce are small. Below, we make approximations for each of the unknown terms in equations (2.12) and (2.13) based upon this assumption, treating each term in turn.

3.4.1 Dissipative Terms, ϵ_{ij}, $\epsilon_{i\theta}$

Since the large-scale motions are essentially independent of viscosity and since viscosity is important in determining the structure of the small scale turbulence, it seems reasonable to assume that the dissipative terms ϵ_{ij} and $\epsilon_{i\theta}$ are isotropic. Now, isotropy requires that properties remain constant following a reversal of any co-ordinate. However, the term $\overline{\frac{\partial v_i}{\partial x_j}\frac{\partial \theta}{\partial x_j}}$ changes sign if the co-ordinates x_i are reversed, indicating that these correlations are not isotropic, contrary to our assumption of high Reynolds number flow. Hence, the only value that the $\epsilon_{i\theta}$ can take is zero:

$$\epsilon_{i\theta} \equiv \left(\frac{\Gamma}{\rho} + \nu\right) \overline{\frac{\partial v_i}{\partial x_j}\frac{\partial \theta}{\partial x_j}} = 0. \tag{3.27}$$

The dissipation terms ϵ_{ij} must also be isotropic. In this case, we must have $i = j$ (no summation), and we can write:

$$\epsilon_{ij} = \frac{2}{3}\,\epsilon\,\delta_{ij} \tag{3.28}$$

where,

$$\epsilon = \nu \overline{\frac{\partial v_i}{\partial x_j} \frac{\partial v_i}{\partial x_j}}. \tag{3.29}$$

We note that this definition of ϵ is identical to that of section 3.1. In order to model this quantity, therefore, we use the equation representing its transport, equation (3.19) of sub-section 3.2.

3.4.2 Pressure-strain and Pressure-scalar Correlations, $\Phi_{ij}, \Phi_{i\theta}$

The pressure strain correlations are important in promoting isotropy. The cross terms in the Reynolds stress tensor are limited only by these correlations, since the quantities ϵ_{ij} are zero for $i \neq j$ (see above). The Φ_{ij} thus remove contributions from $\overline{v_i v_j}$ if $i \neq j$, whilst these terms do not affect the turbulent kinetic energy. Instead, they serve to evenly distribute the diagonal elements $\overline{v_i v_i}$ (no summation) so that these three quantities are equal (Hinze, 1959).

Many models have been proposed for the pressure-strain terms. We will only present a summary here and for more information, readers are referred to Launder (1987), where an excellent review of this subject can be found. The starting point of all models is the consideration of a Poisson equation in the pressure fluctuation. This is obtained by taking the divergence of equation (2.2) and subtracting the divergence of equation (2.10), resulting in

$$\frac{1}{\rho} \frac{\partial^2 p}{\partial x_i^2} = \frac{\partial^2}{\partial x_i \partial x_j} (v_i v_j - \overline{v_i v_j}) + 2 \frac{\partial V_i}{\partial x_j} \frac{\partial v_j}{\partial x_i} + \beta g_i \frac{\partial \theta}{\partial x_i}. \tag{3.30}$$

Taking the usual solution to Poisson's equation, multiplying through by $\partial v_i / \partial x_j$ and time-averaging gives us:

$$\begin{aligned} \overline{\frac{p}{\rho} \frac{\partial v_i}{\partial x_j}} &= \frac{1}{4\pi} \int_{\tau'} \left[\overline{\left(\frac{\partial^2 (v_m v_n)}{\partial x_m \partial x_n} \right)' \frac{\partial v_i}{\partial x_j}} + 2 \left(\frac{\partial V_m}{\partial x_n} \right)' \overline{\left(\frac{\partial v_n}{\partial x_m} \right)' \frac{\partial v_i}{\partial x_j}} \right. \\ &\quad \left. + \beta g_m \overline{\left(\frac{\partial \theta}{\partial x_m} \right)' \frac{\partial v_i}{\partial x_j}} \right] \frac{1}{(x_k - x_k')} d\tau'. \end{aligned} \tag{3.31}$$

Here, a prime indicates that the quantity is to be evaluated at the co-ordinate vector x'_k, whereas all other terms are evaluated at x_k and the integration is carried out over a volume $\tau'(x'_k)$.

This equation demonstrates the processes responsible for the pressure-strain correlations and is very important for this reason. All approximations to the Φ_{ij} must be based upon these processes, and it assumed that this will also be true for the pressure-scalar terms, $\Phi_{i\theta}$. There appear to be three agencies responsible for these correlations and these involve: (i) derivatives of Reynolds stresses, (ii) a mean strain, and (iii) a buoyancy force. On this basis, it seems reasonable to write:

$$\begin{aligned} \Phi_{ij} &= \Phi_{ij1} + \Phi_{ij2} + \Phi_{ij3} \\ \Phi_{i\theta} &= \Phi_{i\theta 1} + \Phi_{i\theta 2} + \Phi_{i\theta 3}, \end{aligned} \tag{3.32}$$

where Φ_{ij1}, $\Phi_{i\theta 1}$ etc. represent contributions to Φ_{ij} and $\Phi_{i\theta}$ respectively due to each of the processes discussed above.

Rotta (1951) appears to have been the first to attempt an approximation of the term Φ_{ij1}. Even today, his model is adopted in nearly all calculations and is:

$$\Phi_{ij1} = -c_1 \frac{\epsilon}{k} \left(\overline{v_i v_j} - \frac{2}{3} \delta_{ij} k \right). \tag{3.33}$$

Where, c_1 is a constant. The equation is valid for $i = j$, in which case $\Phi_{ij1} = 0$ as required. The constant factor 2/3 is used in order to reflect the isotropy of the diagonal terms of the Reynolds stress tensor. If the number of dimensions were reduced from three to two, then this factor would be replaced by 1. In deriving this equation, Rotta suggested that a return to isotropy must be proportional to the level of anisotropy.

A similar model for $\Phi_{i\theta 1}$ was proposed by Monin (1965) and is:

$$\Phi_{i\theta 1} = -c_{1\theta} \frac{\epsilon}{k} \overline{v_i \theta}, \tag{3.34}$$

where $c_{1\theta}$ is again a constant.

Contributions due to the mean shear are generally modelled by the so-called isotropization of production model, in which

$$\Phi_{ij2} = -c_2 \left(P_{ij} - \frac{1}{3} P_{kk} \delta_{ij} \right). \tag{3.35}$$

The idea behind this model is that the production due to a mean shear must be made isotropic by terms such as Φ_{ij2} and was first considered by Naot et al. (1970) (also see Launder et al., 1975). An analogy to this model can easily be made so that the term $\Phi_{i\theta 2}$ can be approximated. The corresponding equation is then

$$\Phi_{i\theta 2} = c_{2\theta} \overline{v_j \theta} \frac{\partial V_i}{\partial x_j}. \tag{3.36}$$

Here, as before, c_2 and $c_{2\theta}$ are constants.

Finally, the buoyancy terms $\Phi_{ij3}, \Phi_{i\theta 3}$ can be modelled according to Launder (1975) as:

$$\Phi_{ij3} = -c_3 (G_{ij} - \frac{1}{3} \delta_{ij} G_{kk}) \tag{3.37}$$

$$\Phi_{i\theta 3} = - c_{3\theta} G_{i\theta}, \tag{3.38}$$

where c_3 and $c_{3\theta}$ are constants. The values of the various constants appearing in these equations can be found in Gibson and Launder (1978).

3.4.3 Diffusive terms, $d_{ij}, d_{i\theta}$

The diffusive terms are the most difficult to model, since the behaviour of the different contributions to these terms is little understood. At present, the only reasonable method appears to be that suggested in Launder (1987).

The method is known as the generalized gradient diffusion hypothesis, and involves approximating unknown correlations of the form $\overline{v_k \chi_{diff}}$ (where χ_{diff} represents a term in the diffusion of the quantity $\overline{\chi}$) by writing:

$$\overline{v_k \chi_{diff}} = -\frac{c_\mu}{\sigma_\chi} \frac{k}{\epsilon} \overline{v_k v_l} \frac{\partial \overline{\chi}}{\partial x_l}. \tag{3.39}$$

Here, c_μ and σ take the definitions of section 3.1.

Often, researchers prefer to use a less complicated form known as simple gradient diffusion. Here, the correlation $\overline{v_k v_l}$ is replaced by the turbulent kinetic energy k. This results in an approximation to the diffusion which is computationally less expensive than the full form given above. However, it has the disadvantage of being less general, since it no longer contains the "cross-stream" diffusion terms of the form

$$\frac{\partial}{\partial x_m} \left(\frac{c_\mu}{\sigma_\chi} \frac{k}{\epsilon} \overline{v_m v_n} \frac{\partial \overline{\chi}}{\partial x_n} \right), \tag{3.40}$$

where we take $m \neq n$ and $m, n = 1, 2, 3$.

The simple gradient diffusion hypothesis is given by:

$$\overline{v_k \chi_{diff}} = -\frac{c_\mu}{\sigma_\chi} \frac{k^2}{\epsilon} \frac{\partial \overline{\chi}}{\partial x_k}, \tag{3.41}$$

The quantity $c_\mu k^2/\epsilon$ is of course the turbulent eddy viscosity introduced in section 3.1. This method of modelling the diffusion is thus equivalent to that of the $k - \epsilon$ model, where the sum of a triple-velocity correlation and a pressure-velocity correlation were assumed to behave in a similar manner to a molecular viscosity term. In section 4, we will use the simple gradient diffusion when modelling the turbulent diffusion, since it is analytically less cumbersome than the generalised version.

If we now consider the diffusion of the Reynolds stresses, we take $\chi_{diff} = (v_i v_j + p \delta_{kj} / \rho + p \delta_{ik} / \rho)$ and $\chi = v_i v_j$. The generalised gradient diffusion hypothesis then gives:

$$\overline{\frac{v_k}{\rho}\left(\rho\, v_i\, v_j + p\,\delta_{ik} + p\,\delta_{jk}\right)} = -\frac{c_\mu}{\sigma_{rs}}\,\frac{k}{\epsilon}\,\overline{v_k\, v_l}\,\frac{\partial\,\overline{v_i\, v_j}}{\partial\, x_l}, \tag{3.42}$$

where σ_{rs} is a turbulent Prandtl number for the Reynolds stresses.

In the case of the unknown correlations in $d_{i\theta}$, we have

$$\overline{v_k\, v_i\, \theta} + \Gamma\,\overline{\theta\,\frac{\partial\, v_i}{\partial\, x_k}} + \nu\,\overline{v_i\,\frac{\partial\,\theta}{\partial\, x_k}} = -\frac{c_\mu}{\sigma_\theta}\,\frac{k}{\epsilon}\,\overline{v_k\, v_l}\,\frac{\partial\,\overline{v_i\,\theta}}{\partial\, x_l}. \tag{3.43}$$

3.4.4 Buoyancy Term, $G_{i\theta}$.

According to our discussion of section 3.2, the term $G_{i\theta}$ can be written as

$$\overline{f_i\,\theta} = -\beta\, g_i\,\overline{\theta^2}. \tag{3.44}$$

The $G_{i\theta}$ thus contain the unknown correlation $\overline{\theta^2}$ and there are essentially two ways in which to model this term. The first method is to solve the transport equation in $\overline{\theta^2}$, which is obtained by multiplying the thermal energy equation (2.3) by θ and averaging to get:

$$\frac{\partial\,\overline{\theta^2}}{\partial\, t} + V_i\,\frac{\partial\,\overline{\theta^2}}{\partial\, x_i} = -2\,\overline{\theta\, v_i}\,\frac{\partial\,\Theta}{\partial\, x_i} - \frac{\partial}{\partial\, x_i}\left(\overline{v_i\,\theta^2} - \Gamma\,\frac{\partial\,\overline{\theta^2}}{\partial\, x_i}\right) - \Gamma\,\overline{\frac{\partial\,\theta}{\partial\, x_i}\,\frac{\partial\,\theta}{\partial\, x_i}}. \tag{3.45}$$

The first term on the right-hand side of this equation represents production of $\overline{\theta^2}$ and does not need to be approximated. The next two terms represent diffusion and dissipation respectively. They do need to be modelled, and we can do this for the diffusive term by writing, in the usual way,

$$\overline{v_i\,\theta^2} = -\frac{c_\mu}{\sigma_{\theta\theta}}\,\frac{k}{\epsilon}\,\overline{v_i\, v_j}\,\frac{\partial\,\overline{\theta^2}}{\partial\, x_j}, \tag{3.46}$$

where $\sigma_{\theta\theta}$ is a turbulent Prandtl number for $\overline{\theta^2}$.

The dissipation has been modelled by Monin (1965), who assumed that

$$\Gamma \overline{\frac{\partial \theta}{\partial x_i} \frac{\partial \theta}{\partial x_i}} = c_{\theta\theta} \frac{\epsilon}{k} \overline{\theta^2}, \tag{3.47}$$

where $c_{\theta\theta}$ is a constant. The equation in the transport of $\overline{\theta^2}$ becomes:

$$\frac{\partial \overline{\theta^2}}{\partial t} + V_i \frac{\partial \overline{\theta^2}}{\partial x_i} = -2 \overline{\theta v_i} \frac{\partial \Theta}{\partial x_i} + \frac{\partial}{\partial x_i} \left[\left(\frac{c_\mu}{\sigma_{\theta\theta}} \frac{k}{\epsilon} \overline{v_i v_j} + \Gamma \delta_{ij} \right) \frac{\partial \overline{\theta^2}}{\partial x_j} \right] - c_{\theta\theta} \frac{\epsilon}{k} \overline{\theta^2}. \tag{3.48}$$

The second method of modelling $\overline{\theta^2}$ is due to Monin (1965), who assumed that the production of this quantity would be equal to its dissipation. Thus, if we approximate the dissipation as before, we can write:

$$-\overline{v_i \theta} = \Gamma \overline{\frac{\partial \theta}{\partial x_i} \frac{\partial \theta}{\partial x_i}} \approx c_{\theta\theta} \frac{\epsilon}{k} \overline{\theta^2}. \tag{3.49}$$

Hence, if $c'_{\theta\theta} = 1/c_{\theta\theta}$, then

$$\overline{\theta^2} = -c'_{\theta\theta} \frac{k}{\epsilon} \overline{v_i \theta} \frac{\partial \Theta}{\partial x_i}. \tag{3.50}$$

In this report, we choose to use the transport equation in order to model $\overline{\theta^2}$ for two related reasons. Firstly, Monin's (1965) model does not take into account diffusive or transient behaviour of $\overline{\theta^2}$, whereas we lose no generality in using the transport equation. Secondly, since we are dealing with a full Reynolds stress closure, we wish to make as few approximations as possible.

We can now re-write the transport equations (2.12) and (2.13) of section 2 and include the equations in $\overline{\theta^2}$ and ϵ. With all the above approximations, these equations are:

Reynolds stress equation:

$$\frac{\partial \overline{v_i v_j}}{\partial t} + V_k \frac{\partial \overline{v_i v_j}}{\partial x_k} = -\left(\overline{v_i v_k} \frac{\partial V_j}{\partial x_k} + \overline{v_j v_k} \frac{\partial V_i}{\partial x_k} \right) - \beta \left(g_i \overline{v_j \theta} + g_j \overline{v_i \theta} \right)$$
$$- c_1 \frac{\epsilon}{k} \left(\overline{v_i v_j} - \frac{2}{3} \delta_{ij} k \right) - c_2 \left(P_{ij} - \frac{1}{3} \delta_{ij} P_{kk} \right)$$
$$- c_3 \left(G_{ij} - \frac{1}{3} \delta_{ij} G_{kk} \right)$$
$$+ \frac{\partial}{\partial x_k} \left[(\nu \delta_{kl} + \frac{c_\mu}{\sigma_{rs}} \frac{k}{\epsilon} \overline{v_k v_l}) \frac{\partial \overline{v_i v_j}}{\partial x_l} \right] - 2 \epsilon \delta_{ij} \quad (3.51)$$

Scalar-flux equation:

$$\frac{\partial \overline{v_i \theta}}{\partial t} + V_j \frac{\partial \overline{v_i \theta}}{\partial x_j} = -\left(\overline{v_i v_j} \frac{\partial \Theta}{\partial x_j} + \overline{v_j \theta} \frac{\partial V_i}{\partial x_j} \right) - \beta g_i \overline{\theta^2}$$
$$- c_{1\theta} \frac{\epsilon}{k} \overline{v_i \theta} + c_{2\theta} \overline{v_j \theta} \frac{\partial V_i}{\partial x_j} - c_{3\theta} G_{i\theta}$$
$$+ \frac{\partial}{\partial x_k} \left[(\delta_{kl} (\Gamma + \nu) + \frac{c_\mu}{\sigma_\theta} \frac{k}{\epsilon} \overline{v_k v_l}) \frac{\partial \overline{v_i \theta}}{\partial x_l} \right] \quad (3.52)$$

Equation in $\overline{\theta^2}$:

$$\frac{\partial \overline{\theta^2}}{\partial t} + V_i \frac{\partial \overline{\theta^2}}{\partial x_i} = -2 \overline{\theta v_i} \frac{\partial \Theta}{\partial x_i} + \frac{\partial}{\partial x_i} \left[(\Gamma \delta kl \frac{c_\mu}{\sigma_{\theta\theta}} \frac{k}{\epsilon} \overline{v_i v_j}) \frac{\partial \overline{\theta^2}}{\partial x_j} \right] - c_{\theta\theta} \frac{\epsilon}{k} \overline{\theta^2} \quad (3.53)$$

Dissipation equation:

$$\frac{\partial \epsilon}{\partial t} + V_j \frac{\partial \epsilon}{\partial x_j} = \frac{\partial}{\partial x_i} \left[\left(\nu \delta_{ij} + \frac{c_\mu}{\sigma_\epsilon} \frac{k}{\epsilon} \overline{v_i v_j} \right) \frac{\partial \epsilon}{\partial x_j} \right] + c_{1\epsilon} \frac{\epsilon}{k} \overline{v_i v_j} \frac{\partial V_i}{\partial x_j} - c_{2\epsilon} \frac{\epsilon^2}{k}$$
$$- c_{3\epsilon} c_{1\epsilon} \frac{\epsilon}{k} \beta g_i \overline{v_i \theta} \quad (3.54)$$

and the model is now closed.

The amount of computational work required for a Reynolds stress closure of this type is increased dramatically over that required for a $k - \epsilon$ model. In the former, we must solve sixteen simultaneous partial differential equations: five in the transport of the mean quantities, six in the transport of the Reynolds stresses, three in the transport of the scalar heat flux and one each for the quantities $\overline{\theta^2}$ and ϵ. This compares with only seven equations for the $k - \epsilon$ model, with a decrease of more than a factor of two.

3.5 Large Eddy Simulation

The large eddy simulation involves modelling the large scale turbulence. The techniques used are so different from the closures previously discussed that a full discussion of them would require a separate report. However, we will briefly mention the basic method just for completeness. The technique is analogous to that of averaging the transport equations, as was done in section 2. However, in this case, the variables describing the flow are separated not into a mean and fluctuating quantity, but rather into large- and small-scale components. We can write the velocity $\tilde{V}_i$, for example, as

$$\tilde{V}_i = \overline{V}_i + V_i' \tag{3.55}$$

where $\tilde{V}_i$ represents the fluid velocity (see section 2), $\overline{V}_i$ is a large-scale component of the turbulent velocity and V_i' is a small-scale turbulent velocity. The quantity $\overline{V}_i$ can be separated from the small scale velocity by taking a convolution of $\tilde{V}_i$ with a filter which has the relevant cut-off in its spectrum:

$$\overline{V_i} = \int G(x - x')\, \tilde{V}_i \, dx' \tag{3.56}$$

where x and x' are co-ordinate vectors and $G(x - x')$ is the required filter. Biringen and Reynolds (1981) used a Gaussian filter of the form

$$G(x - x') = \left(\frac{\alpha}{\delta}\right)^3 exp\left[-\pi\, \alpha^2\, (x - x')^2 / \Delta^2\right] \tag{3.57}$$

where α is a constant and Δ is the required filter width. Equation (3.55) is substituted into equations (2.1) to (2.3) of section 2, and in order to complete the model, the small-scale quantities are written in terms of the large scale variables. A coefficient of kinematic eddy-viscosity, ν_t', is often employed in order to accomplish this and a sub-grid scale model is introduced. In this way, an exchange of energy from the larger to the smaller scales is represented. This so-called 'energy cascade' is characteristic of turbulence (cf. Bradshaw, 1976) and in some sense is a dissipation imposed upon the larger eddies. The quantity ν_t' then represents the coefficient required in order to model such a dissipation.

The large eddy simulation would possibly be of use in modelling strongly-convective flows of the type under consideration in this report; however, little work has been done with this application in mind. We will therefore defer any further analysis of the subject. Further details of the technique of large eddy simulation may be found in, for example, Clark et al. (1979) or Biringen and Reynolds (1981).

3.6 Direct Simulation

Direct simulation is the final method of determining a turbulent flow that we shall discuss in this section. The method does not depend upon deriving a turbulence closure scheme, but involves a direct numerical solution to the basic equations describing the flow (equations (2.1) to (2.3) in section 2). The reasoning is, of course, that the solutions which one obtains must implicitly contain information regarding the turbulence and, once these solutions have been found, no further work need be done.

However, the method as yet does not provide information regarding the structure of fine-scale turbulence. The reason for this is that, in order to resolve such structure, very fine grids are required on which to solve the equations. Schumann (1987), estimates that if the amount of available computational time is T, then the number of grid points, N must be limited by $N \sim T^{\frac{1}{4}}$, where N is an estimate for the solution to one variable and in one direction. This estimate must vary, however, depending on the computer. The use of super-computers would be expected to increase this value of N.

In order to resolve the small-scale turbulence Schumann (1987) supposes that one would require a grid of 512^3 points. Grötzbach (1986a) studied Rayleigh-Benard convection using direct-simulation and a $64 \times 64 \times 32$ grid. He reports that 38.2 hours of IBM-3033 cpu time were used. This size of grid does not, however, model the fine-scale turbulence, Furthermore, the Rayleigh numbers used are only of order 10^6 - many orders of magnitude lower than those required in our application. Intuitively, one would expect that larger Rayleigh numbers implies the presence of turbulence on a small scale. It is expected therefore that one would require finer grids than those of Grötzbach. We conclude, therefore, that the direct simulation technique is not of relevance to our particular problem, since it is likely to take too much computer time and cannot at present provide us with the necessary details of the structure of small-scale turbulence. We will not mention this method further in this report.

4. Application of Closures to Strongly-Convective Flows

In this section, we examine if the turbulence models of the previous section can be applied to the problem of a high Rayleigh number flow. We emphasize at this stage that the analysis of this section is very idealistic, with many assumptions being made. Furthermore, it will not be clear whether or not many of the more complicated physical processes can be modelled in this analysis. We only wish to show whether a turbulent solution exists in a particular situation where there is no mean flow. A general flow of this type will not be examined.

In establishing whether turbulence closure schemes are relevant to this type of flow, one must consider full-Reynolds stress closures since these are the most general of the second-order models. If these do not model the flow more successfully than a Nusselt number correlation, then no lower-order closure will be able to do so, and there is no further point in examining turbulence modelling. If the Reynolds stress closure is successful, then one should also study two-equation or, perhaps, lower-order schemes, since these may be more favourable than a Reynolds-stress closure because much less computational time is used in solving the equations which describe the turbulence.

Therefore, the models we will be studying are the $k - \epsilon$ and the full Reynolds stress closure. We need not include the algebraic-stress model for several reasons. These models are less general than a full Reynolds stress model, although of a higher-order than the $k - \epsilon$ model. The former of these should contain details of all the relevant physical processes, whilst the latter is simpler to work with, both analytically and computationally. The algebraic stress model, however, comes somewhere between the two.

Furthermore, by studying the equations describing this closure, it is not obvious how this method would be preferable over the $k - \epsilon$ model. In our application, we assume that the mean flow is zero. In this situation, the

ASM provides exactly the same processes for generating the scalar heat flux as in the $k - \epsilon$ model, with the addition of terms in $\overline{v_i v_j}$ and $\overline{\theta^2}$. Physically, it is not clear why these terms should be the only ones which contribute, and the central assumption in generating these models still appears to be that the main force in driving the turbulence is shear, rather than buoyancy. (This is not, of course, unreasonable, since almost all of the applications of these models deal with flows in which the shear has a strong influence on the turbulence.) Therefore, we will not consider algebraic stress type models any further in this report. We should perhaps emphasize, however, that algebraic stress models have been very successful in modelling other types of flow, and the comments made here should not be applied to these situations.

In modelling a highly-convective flow we make several assumptions. The first is the assumption of a zero mean velocity, in accordance with the discussion of section 2 and is based upon experimental results. This simplifies the equations significantly, with the advective terms and the P_{ij} being identically zero. Obviously, before making this assumption, it is necessary to ensure that the flow is turbulent, so that the mean flow can be separated from the turbulent fluctuations. In this case, it is assumed that any velocities which are generated due to the convection will not consist of an overall mean, but will be due only to random motion. Secondly, we assume that the flow is two-dimensional, with one vertical and one horizontal direction being given by y and x respectively. This is for mathematical simplicity and is in fact contrary to our understanding of the structure of turbulence, since turbulence is essentially a three-dimensional phenomenon (see, for example, Tennekes and Lumley, 1972). More work is required regarding this subject, to establish whether the results of this report are significantly affected by the neglect of the third spatial variable. Thirdly, we physically require that the gravitational acceleration g_i acts in the downward direction only and can be written as $g_i = -g$. We also assume that, for the smallest scales of motion present, the turbulent kinetic energy k is isotropic, so that $k = \overline{v_i^2}$ for $i = 1$ or 2 (no summation), in accordance with the discussions of section 3. Finally, in the next two sub-sections we make the assumption of zero diffusion. In shear-driven flows, this would be reasonable, since the eddies which characterise the turbulence are generated mainly by shear. However, the assumption is again made here for mathematical simplicity and in order to illustrate the importance of diffusion in convection-driven turbulence. Therefore, we begin by looking at the $k - \epsilon$ and Reynolds stress models neglecting diffusion, and go on later to consider these models with diffusion. For this purpose, we use the simple gradient diffusion hypothesis outlined in section 3.4.3.

4.1 The $k - \epsilon$ model without diffusion

The closure scheme which we require is given in section 3.2, equations (3.18) and (3.19). However, we vary this a little, by not using the Boussinesq hypothesis to model the scalar heat flux, $\overline{\theta\, v_i}$ (equation (3.17)) and $\overline{\theta^2}$ (equation (3.50)). There are several reasons for not wanting to use the Boussinesq hypothesis. Although most of them are not applicable here, we will mention them at this point, since they will be required later. The first reason is concerned with the mean temperature gradient. If this gradient is present in only one direction, then information regarding the scalar heat flux perpendicular to this direction will be lost. Secondly, the hypothesis has been shown to be inconsistent with the boundary layer solutions of George and Capp (1979). If we assume that the solutions of George and Capp are correct, then we must also conclude that the Boussinesq hypothesis cannot be used in this case. Finally, the hypothesis contains no information regarding the diffusion or dissipation of the scalar heat flux, whereas we see later that the former of these processes at least ought to be included in a convective fluid with no mean flow. Therefore, this author feels that it is better to use the transport equations for these quantities, especially since this is an analytic treatment and nothing can be gained by their neglect.

With the assumption of zero mean flow ($V_i = 0$) and no diffusion, the equations describing the transport of the turbulence are:

$$\frac{\partial k}{\partial t} = \beta\, g\, \overline{\theta\, v_2} - \epsilon \tag{4.1}$$

$$\frac{\partial \overline{v_i\, \theta}}{\partial t} = -k\, \delta_{ij} \frac{\partial \Theta}{\partial x_j} + (1 - c_{3\theta})\beta\, g\, \overline{\theta^2}\, \delta_{i2} - c_{1\theta} \frac{\epsilon}{k} \overline{v_i\, \theta} \tag{4.2}$$

$$\frac{\partial \overline{\theta^2}}{\partial t} = -2\, \overline{v_i\, \theta} \frac{\partial \Theta}{\partial x_i} - c_{\theta\theta} \frac{\epsilon}{k} \overline{\theta^2} \tag{4.3}$$

$$\frac{\partial \epsilon}{\partial t} = c_{1\epsilon}\, c_{3\epsilon} \frac{\epsilon}{k} \beta\, g\, \overline{v_2\, \theta} - c_{2\epsilon} \frac{\epsilon^2}{k}. \tag{4.4}$$

In deriving the second of these equations, we have approximated the Reynolds stress by the modified Boussinesq hypothesis, equation (3.10). This illustrates a very important point. By using the Boussinesq hypothesis with no mean flow, we are effectively saying that all of the Reynolds shear stresses are zero, since the only non-zero components of the stresses are $k\,\delta_{ij}$. This is clearly not the case. Even though the re-distribution terms Φ_{ii} attempt to destroy the Reynolds stresses, these quantities do appear in the terms representing the production of the scalar heat fluxes (see the full Reynolds stress closure) and in neglecting them, we may be losing some important physics. (In the case of a zero mean flow, the Reynolds stresses would presumably be produced through the action of the mean temperature gradient. A model for them should therefore be based upon such a mechanism.) The fact that the Reynolds stresses are zero, therefore, must be a consequence of an incorrect closure for this particular problem.

We can examine if a non-trivial turbulent solution exists by studying the steady-state solutions of the above equations. Therefore, we set all derivatives with respect to time equal to zero and write the equations in terms of components to get:

$$\beta\, g\, \overline{v_2\,\theta} - \epsilon = 0 \tag{4.5}$$

$$-k\,\frac{\partial\,\Theta}{\partial\,x} - c_{1\theta}\,\frac{\epsilon}{k}\,\overline{v_1\,\theta} = 0 \tag{4.6}$$

$$-k\,\frac{\partial\,\Theta}{\partial\,y} + (1 - c_{3\theta})\,\overline{\theta^2}\,g\,\beta - c_{1\theta}\,\frac{\epsilon}{k}\,\overline{v_2\,\theta} = 0 \tag{4.7}$$

$$-2\,\overline{v_1\,\theta}\,\frac{\partial\,\Theta}{\partial\,x} - 2\,\overline{v_2\,\theta}\,\frac{\partial\,\Theta}{\partial\,y} - c_{\theta\theta}\,\frac{\epsilon}{k}\,\overline{\theta^2} = 0 \tag{4.8}$$

$$c_{3\epsilon}\,c_{1\epsilon}\,\beta\,g\,\overline{v_2\,\theta}\,\frac{\epsilon}{k} - c_{2\epsilon}\,\frac{\epsilon^2}{k} = 0. \tag{4.9}$$

Equation (4.5) tells us that $\beta\, g\, \overline{v_2\,\theta} = \epsilon$. Substitution of this result into equation (4.9) gives $\epsilon = 0$, where we assume that $c_{3\epsilon}\,c_{1\epsilon} \neq c_{2\epsilon}$. Equation (4.5) then gives $\overline{v_2\,\theta} = 0$. These quantities being zero implies that all other turbulent correlations are zero, providing that the mean temperature gradient is a function of both x and y.

We may also examine circumstances where the mean temperature is a function of only x or y. The first of these is trivial and again suggests that all turbulent quantities are zero. In the case when the gradient is a function of y only, we find that ϵ and $\overline{v_2\,\theta}$ are zero, as before. However, $\overline{v_1\,\theta}$ is now arbitrary, since ϵ and $\partial\,\Theta/\partial\,x$ are identically zero. We may take $\overline{v_1\,\theta}$ to be zero also, without loss of generality. The final two quantities are related through equation (4.7), which gives,

$$k\,\frac{\partial\,\Theta}{\partial\,y} = \beta\,g\,(\,1 - c_{3\theta}\,)\,\overline{\theta^2}. \tag{4.10}$$

We know that $g > 0$, and if we assume that $c_{3\theta}$ is a universal constant which is less than unity (see, for example, Bradshaw et al., 1981) and that the equation of state is such that $\beta > 0$, then there are two possibilities:

(i) $\partial\,\Theta\,/\,\partial\,y < 0$

In this case, we have that either k or $\overline{\theta^2}$ must be negative definite. However, this is contrary to physical reasoning, since these quantities correspond to a summation of squared turbulent quantities, and physically these ought not to be negative. The only value that k or $\overline{\theta^2}$ can take, therefore, is again zero.

(ii) $\partial\,\Theta\,/\,\partial\,y > 0$

This is a stable temperature stratification. Again, one would expect the quantities k and $\overline{\theta^2}$ to be zero, since there is now no convection to drive the turbulence. For example, if one considers a box of fluid with heated top and cooled bottom, then a fluid with initial constant temperature will merely re-organise itself so that it is stably stratified in temperature. Any perturbation which develops as it does this will die away with time. Therefore the steady-state must be the one with $k,\ \overline{\theta^2} \equiv 0$. However, this is an intuitive conclusion, and apparently cannot be proved in this analysis, since both k and $\overline{\theta^2}$ appear to be arbitrary. Note, however, that if one had used the original Boussinesq hypothesis, equation (3.9) of section 3.1, then the first term on the left-hand side of equations (4.6) and (4.7) would be zero. The "expected" value of $\overline{\theta^2} = 0$ would then follow automatically, regardless of the sign of the temperature gradient.

These results show that the model must be incorrect, since we know from experimental evidence that convective flows can be turbulent. We conclude, therefore, that this turbulence closure is not useful in describing this type of flow.

4.2 Full Reynolds stress model without diffusion

The previous model was unsuccessful in showing evidence of steady-state turbulence with no mean flow. If this closure is similarly unproductive, then we have established that we must at best include diffusion in the model, and at worst have to invent a new closure for these flows. With the assumptions described earlier, the steady-state form of equations (3.51) to (3.54) of section 3 is:

$$\beta\, g\, \overline{v_2\,\theta} - \epsilon = 0 \tag{4.11}$$

$$(1 - c_3)\,\beta\, g\, \overline{v_1\,\theta} - c_1\,\frac{\epsilon}{k}\,\overline{v_1\,v_2} = 0 \tag{4.12}$$

$$-k\,\frac{\partial\,\Theta}{\partial\,x} - \overline{v_1\,v_2}\,\frac{\partial\,\Theta}{\partial\,y} - c_{1\theta}\,\frac{\epsilon}{k}\,\overline{v_1\,\theta} = 0 \tag{4.13}$$

$$-k\,\frac{\partial\,\Theta}{\partial\,y} - \overline{v_1\,v_2}\,\frac{\partial\,\Theta}{\partial\,x} - c_{1\theta}\,\frac{\epsilon}{k}\,\overline{v_2\,\theta} + (1 - c_{3\theta})\,\beta\, g\,\overline{\theta^2} = 0 \tag{4.14}$$

$$-2\,\overline{\theta\,v_2}\,\frac{\partial\,\Theta}{\partial\,y} - 2\,\overline{\theta\,v_1}\,\frac{\partial\,\Theta}{\partial\,x} - c_{\theta\theta}\,\frac{\epsilon}{k}\,\overline{\theta^2} = 0 \tag{4.15}$$

$$c_{1\epsilon}\,c_{3\epsilon}\,\beta\, g\,\overline{v_2\,\theta}\,\frac{\epsilon}{k} - c_{2\epsilon}\,\frac{\epsilon^2}{k} = 0. \tag{4.16}$$

The first and last of these equations again indicates that the quantities ϵ and $\overline{v_2\,\theta}$ are both zero which in turn implies that $\overline{v_1\,\theta}$ is also zero. If the mean temperature is dependent upon only x or only y, then we again find that there will be no steady-state turbulence.

If the temperature varies in both directions, we find that k, $\overline{v_i\,v_j}$ and $\overline{\theta^2}$ are indeterminate and are related by

$$c_{3\theta}\,\beta\, g\,\overline{\theta^2}\,\frac{\partial\,\Theta}{\partial\,y} = k\left[\left(\frac{\partial\,\Theta}{\partial\,y}\right)^2 - \left(\frac{\partial\,\Theta}{\partial\,x}\right)^2\right] \tag{4.17}$$

$$-\overline{v_1\,v_2}\,\frac{\partial\,\Theta}{\partial\,y} = k\left(\frac{\partial\,\Theta}{\partial\,x}\right)^2. \tag{4.18}$$

In our application, we are concerned with a pool of molten material confined within a container. The pool is expected experimentally to have a mean flow which is approximately zero. However, if a horizontal temperature gradient exists, then a mean flow should appear, since there would be no term to balance the subsequent horizontal forces. In other words, the mean flow would be due to a resultant force acting on the fluid. Therefore we take a mean temperature which varies in the vertical direction only. In this case, the turbulence model suggested in this section indicates that no turbulence will occur in this application and we again have a situation in which the turbulence closure does not appear to represent the flow correctly. We should also note that, at the boundaries at least, the dissipation must remain non-zero. If this were not true, then there would be no viscous dissipation to halt the growth of the turbulent kinetic energy in the main part of the flow.

For these reasons we must include diffusion in the closure. In fact, one would presume that diffusion must be included purely on physical grounds anyway. In shear-driven turbulence, there is no need for diffusion to be present, since turbulent energy is transported around the fluid by the action of the mean velocity field upon the Reynolds stresses. In our application, we have no such mechanism and diffusion must be important for this reason. The results of this and the previous sub-section have merely confirmed this hypothesis.

4.3 $k - \epsilon$ model with diffusion

Given a steady-state and the assumptions of previous sections, the equations describing the model are:

$$\beta\, g\, \overline{v_2\, \theta} - \epsilon + \frac{\partial}{\partial x_k}\left[\left(\nu + \frac{c_\mu}{\sigma_k}\frac{k^2}{\epsilon}\right)\frac{\partial k}{\partial x_k}\right] = 0 \quad (4.19)$$

$$-k\,\frac{\partial \Theta}{\partial x} - c_{1\theta}\,\frac{\epsilon}{k}\,\overline{v_1\,\theta} + \frac{\partial}{\partial x_k}\left[\left(\Gamma + \nu + \frac{c_\mu}{\sigma_\theta}\frac{k^2}{\epsilon}\right)\frac{\partial \overline{v_1\,\theta}}{\partial x_k}\right] = 0 \quad (4.20)$$

$$-k\,\frac{\partial \Theta}{\partial y} + (1 - c_{3\theta})\,\overline{\theta^2}\, g\,\beta - c_{1\theta}\,\frac{\epsilon}{k}\,\overline{v_2\,\theta} + \frac{\partial}{\partial x_k}\left[\left(\Gamma + \nu + \frac{c_\mu}{\sigma_\theta}\frac{k^2}{\epsilon}\right)\frac{\partial \overline{v_2\,\theta}}{\partial x_k}\right] = 0 \quad (4.21)$$

$$
-2\,\overline{v_1\,\theta}\,\frac{\partial\,\Theta}{\partial\,x} - 2\,\overline{v_2\,\theta}\,\frac{\partial\,\Theta}{\partial\,y} - c_{\theta\theta}\,\frac{\epsilon}{k}\,\overline{\theta^2}
$$

$$
+\frac{\partial}{\partial\,x_k}\left[\left(\Gamma + \frac{c_\mu}{\sigma_{\theta\theta}}\,\frac{k^2}{\epsilon}\right)\frac{\partial\,\overline{\theta^2}}{\partial\,x_k}\right] = 0 \quad (4.22)
$$

$$
c_{3\epsilon}\,c_{1\epsilon}\,\beta\,g\,\overline{v_2\,\theta}\,\frac{\epsilon}{k} - c_{2\epsilon}\,\frac{\epsilon^2}{k} + \frac{\partial}{\partial\,x_k}\left[\left(\nu + \frac{c_\mu}{\sigma_\epsilon}\,\frac{k^2}{\epsilon}\right)\frac{\partial\,\epsilon}{\partial\,x_k}\right] = 0. \quad (4.23)
$$

These equations are obviously very complicated, and it is not easy to derive any useful physics from them. However, the most important diffusion terms ought to be those in the turbulent kinetic energy and the scalar heat flux. (The scalar heat flux determines the density variation, whilst the density variation influences the velocity field and hence the turbulent kinetic energy.) We can simplify further by working in the regime where the term representing the diffusion of the scalar heat flux is much less important than that in the turbulent kinetic energy equation. We do not wish to know at this point whether such a regime exists, since we are presently concerned with showing that our model can predict turbulence under some conditions. With these assumptions, we have the following, much more manageable set of equations:

$$
\beta\,g\,\overline{v_2\,\theta} - \epsilon + \frac{\partial}{\partial\,x_k}\left[\left(\nu + \frac{c_\mu}{\sigma_k}\,\frac{k^2}{\epsilon}\right)\frac{\partial\,k}{\partial\,x_k}\right] = 0 \quad (4.24)
$$

$$
-k\,\frac{\partial\,\Theta}{\partial\,x} - c_{1\theta}\,\frac{\epsilon}{k}\,\overline{v_1\,\theta} = 0 \quad (4.25)
$$

$$
-k\,\frac{\partial\,\Theta}{\partial\,y} + (1 - c_{3\theta})\,\overline{\theta^2}\,g\,\beta - c_{1\theta}\,\frac{\epsilon}{k}\,\overline{v_2\,\theta} = 0 \quad (4.26)
$$

$$
-2\,\overline{v_1\,\theta}\,\frac{\partial\,\Theta}{\partial\,x} - 2\,\overline{v_2\,\theta}\,\frac{\partial\,\Theta}{\partial\,y} - c_{\theta\theta}\,\frac{\epsilon}{k}\,\overline{\theta^2} = 0 \quad (4.27)
$$

$$
c_{3\epsilon}\,c_{1\epsilon}\,\beta\,g\,\overline{v_2\,\theta}\,\frac{\epsilon}{k} - c_{2\epsilon}\,\frac{\epsilon^2}{k} = 0. \quad (4.28)
$$

Again assuming that the temperature varies in a vertical direction only, eliminating $\overline{v_2\,\theta}$ between (4.24) and (4.26) gives a relationship in $\overline{\theta^2}$. We can substitute this into (4.27) and use (4.28) to derive a pair of simultaneous equations in k and ϵ:

$$\frac{\epsilon}{k}\left[\epsilon\frac{(A-1)}{A}-\frac{\partial}{\partial x_k}\left(\left(\frac{c_\mu}{\sigma_k}\frac{k^2}{\epsilon}+\nu\right)\frac{\partial k}{\partial x_k}\right)\right]=0 \qquad (4.29)$$

$$\left[2\{1-c_{3\theta}\}\{\epsilon-\frac{\partial}{\partial x_k}\left(\left(\frac{c_\mu}{\sigma_k}\frac{k^2}{\epsilon}+\nu\right)\frac{\partial k}{\partial x_k}\right)\}+\epsilon\, c_{\theta\theta}\right]\beta g\frac{\partial\Theta}{\partial y}$$

$$+\,c_{\theta\theta}\,c_{1\theta}\frac{\epsilon^2}{k^2}\{\epsilon-\frac{\partial}{\partial x_k}\left(\left(\frac{c_\mu}{\sigma_k}\frac{k^2}{\epsilon}+\nu\right)\frac{\partial k}{\partial x_k}\right)\}=0, \qquad (4.30)$$

where $A = c_{3\epsilon}\, c_{1\epsilon} / c_{2\epsilon}$.

In deriving these equations, we have been careful not to divide by any correlation, in case that quantity is physically zero. In the limit of zero diffusion, the first of these equations provides us with exactly the same result as in sub-section 4.1 that $\epsilon = 0$, whilst the second vanishes to zero identically (assuming that ϵ goes to zero at least as quickly as k).

Eliminating the k-diffusion term from equations (4.29) and (4.30) allows us to determine ϵ as a function of k, providing that solutions are taken far from regions where k and ϵ are zero. In this case,

$$\epsilon^2 = -k^2\,(2(1-c_{3\theta})+A\,c_{\theta\theta})\,\beta g\frac{\partial\Theta}{\partial y}\,/\,c_{1\theta}\,c_{\theta\theta}. \qquad (4.31)$$

We should note here that a derivation of equation (4.31) does not rely upon the form of the diffusion, the only requirement being that the diffusion be non-zero. It is the inclusion of the diffusive term in equation (4.24) that allows the viscosity to be non-zero. The values generally given for the various constants in equation (4.31) (Bradshaw et al, 1981; Launder, 1987) reveal that they are all greater than zero, and $c_{3\theta} < 1$. Also, the dissipation in equation (4.31) must be positive definite (it is the average of the square of a real quantity) and this will be true only if the temperature gradient in equation (4.31) is negative. This is exactly the situation in which one would expect there to be turbulence, and is the opposite of what we have found in previous sub-sections. However, whether equation (4.31) has any real physical interpretation is uncertain.

Equation (4.29) is also interesting, since it indicates that if ϵ is non-zero, then the diffusion is proportional to the dissipation. This equation is analogous to that of steady-state heat transfer with a sink and represents the diffusion of turbulent kinetic energy to a region where it can be dissipated. Furthermore, we can re-write equation (4.24) in terms of $\overline{v_2\,\theta}$ and the dissipation only and we again find that diffusion is not explicitly present in our system of equations (4.24) to (4.28). Note also that, since we have neglected all other diffusive terms, we should be careful not to place too much emphasis on the above results. However, the inclusion of further diffusion terms should still provide us with a non-zero turbulent solution in the steady-state, since diffusion cannot remove energy from the turbulence. We presume, therefore, that the basic interpretation of equation (4.31) is valid.

However, there are still problems with the model. If we impose the conditions at a surface that the turbulent kinetic energy must be zero, then for reasons of regularity, ϵ must go to zero at least as quickly as k. Furthermore, one finds that the dissipation must go to zero less quickly than k^2, otherwise, the diffusion terms would not be regular (assuming the various gradients of correlations exist). We thus find that $O(k) \leq \epsilon \leq O(k^2)$. This is not what one would expect by studying a power series expansion close to a wall, where one finds that $k \sim O(y^2)$, whilst $\epsilon \sim O(1)$ (cf. Fletcher, 1982).

We can conclude, therefore, that there are again some inconsistencies in this model. This time, the problems seem to be largely due to the selection of correct boundary conditions. There is not room here to fully discuss solutions to this problem and we will return to the subject in a later report.

4.4 Reynolds stress model with diffusion

We will make only a few comments regarding this model, since the equations are far too complicated to derive any useful physics from. Furthermore, the model does not appear to be significantly different from the $k-\epsilon$ model, with only one extra equation in the Reynolds stress $\overline{v_i\,v_j}$ being present. In steady state the equations are:

$$\beta\, g\, \overline{v_2\,\theta} - \epsilon + \frac{\partial}{\partial x_k}\left[\left(\nu + \frac{c_\mu}{\sigma_k}\frac{k^2}{\epsilon}\right)\frac{\partial\, k}{\partial\, x_k}\right] = 0 \qquad (4.32)$$

$$(1 - c_3)\beta g \overline{v_1 \theta} - c_1 \frac{\epsilon}{k} \overline{v_1 v_2} + \frac{\partial}{\partial x_k}\left[\left(\nu + \frac{c_\mu}{\sigma_{rs}} \frac{k^2}{\epsilon}\right) \frac{\partial \overline{v_i v_2}}{\partial x_k}\right] = 0 \qquad (4.33)$$

$$-k \frac{\partial \Theta}{\partial x} - \overline{v_1 v_2} \frac{\partial \Theta}{\partial y} - c_{1\theta} \frac{\epsilon}{k} \overline{v_1 \theta} + \frac{\partial}{\partial x_k}\left[\left(\nu + \Gamma + \frac{c_\mu}{\sigma_\theta} \frac{k^2}{\epsilon}\right) \frac{\partial \overline{v_1 \theta}}{\partial x_k}\right] = 0 \qquad (4.34)$$

$$-k \frac{\partial \Theta}{\partial y} - \overline{v_1 v_2} \frac{\partial \Theta}{\partial x} - c_{1\theta} \frac{\epsilon}{k} \overline{v_2 \theta} + (1 - c_{3\theta})\beta g \overline{\theta^2} + \frac{\partial}{\partial x_k}\left[\left(\nu + \Gamma + \frac{c_\mu}{\sigma_\theta} \frac{k^2}{\epsilon}\right) \frac{\partial \overline{v_2 \theta}}{\partial x_k}\right] = 0 \qquad (4.35)$$

$$-2\overline{\theta v_2} \frac{\partial \Theta}{\partial y} - 2\overline{\theta v_1} \frac{\partial \Theta}{\partial x} - c_{\theta\theta} \frac{\epsilon}{k} \overline{\theta^2} + \frac{\partial}{\partial x_k}\left[\left(\Gamma + \frac{c_\mu}{\sigma_{\theta\theta}} \frac{k^2}{\epsilon}\right) \frac{\partial \overline{\theta^2}}{\partial x_k}\right] = 0 \qquad (4.36)$$

$$c_{1\epsilon}\, c_{3\epsilon} \beta g \overline{v_2 \theta} \frac{\epsilon}{k} - c_{2\epsilon} \frac{\epsilon^2}{k} + \frac{\partial}{\partial x_k}\left[\left(\nu + \frac{c_\mu}{\sigma_\epsilon} \frac{k^2}{\epsilon}\right) \frac{\partial \epsilon}{\partial x_k}\right] = 0. \qquad (4.37)$$

In studying these equations, we find that the same problems regarding the selection of correct boundary conditions are still present.

The difficulties could be due to the use of an incorrect set of approximations in closing the equations, or it could really be that we do not understand what the boundary conditions should be. In the former case, the only terms which appear to have been unreasonably approximated are those representing diffusion and dissipation. We have seen, however, that the $k - \epsilon$ model does appear to allow steady-state turbulence, as long as solutions are taken away from a wall, so that neither k or ϵ are expected to be zero. (This is consistent with the assumption which we have made previously that the Reynolds number is high, so that the small-scale motion is dependent upon viscosity.) We conclude, therefore, that the models are not valid close to a wall. A possible approach to this problem will be examined in a subsequent report, where we will study the expected boundary layer close to the wall. This has already been accomplished in a paper by George and Capp (1979) and our later report will review this work.

5. Summary and Conclusions

In this report, we have set out to investigate whether currently available turbulence closure schemes are applicable to a strongly-convecting flow. In section 3, we summarised several closures of different complexity, and in section 4, they were applied to the convective flow in the limit of steady-state and with the assumption of a zero mean flow.

We have discovered that there are at least two major problems with the models which we have examined. The first is the most important and is concerned with the selection of the correct boundary conditions. In a shear-driven turbulence, one would usually choose the conditions at a surface that turbulent velocities be zero there. However, we have seen that the assumption of a zero mean velocity field (see section 2) precludes this choice, since the steady-state must then be the one with a trivial solution for the turbulent correlations. In order to get round this problem, we decided that it is necessary to calculate the flow in a boundary layer close to the walls of the fluid's container. The reasoning is, as was pointed out in sections 2 and 4, that the turbulent flow is expected to posses a thin boundary layer, whose mean flow should not be zero. In this situation, one would be expected to be able to use the usual boundary conditions at a surface.

This brings us to the second problem with turbulence models. Given such a boundary layer, we wish to know how the turbulence feeds off it. We assume that the process must involve a diffusive action. In many turbulence closures, diffusion is left out of the equations altogether, since its effects are expected to be small. This will almost certainly be true in shear-driven turbulence where the mean flow dominates over the diffusion. In our application, however, we have pointed out that this is not the case, and we must be concerned with developing a "reasonable" diffusion model. At this point, we should ask if the modelled diffusion suggested in this report would be successful in modelling the true, physical process. The answer to this question is uncertain at present. Thompson et al. (1985) and Wilkes and Thompson (1986) investigated the double-glazing problem using the boundary layer equations of George and Capp (1979). However, they do not report on how well the diffusion is modelled. Furthermore, for the numerical examinations that have been attempted, there is little experimental evidence with which to compare the results.

We have thus been able to demonstrate two major defects in current turbulence modelling, as applied to a strongly-convecting flow. Firstly, we need to determine a physically meaningful diffusion model, which is not based on a mean flow. Secondly, we must derive a set of boundary layer equations which ought to be at least analogous to those of George and Capp (1979). If the $k - \epsilon$ model of section 4 is to be used, then we also ought to include a model for the generation of the Reynolds stresses, in the absence of a mean flow. In neglecting such a model, we must be losing some knowledge of the physical processes which contribute to the turbulence, and the inclusion of Reynolds stresses must be important for this reason.

We conclude by commenting upon the applicability of current turbulence models to strong natural convective flows. As we have stressed many times throughout this report, the currently available "state of the art" turbulence models are based upon the assumption that the turbulence is driven by a mean shear. There are several provisos regarding such models:

(i) The body forces must be kept in the model.

(ii) A reasonable model must be found for the turbulent correlations $\overline{v_i v_j}$, $\overline{v_i \theta}$ and $\overline{\theta^2}$. The first two of these would be expected to be the most important. Models of these terms must not be based solely on a mean velocity and ought to have some diffusive properties.

(iii) Finally, solutions must be calculated in a boundary layer in order to provide boundary conditions for the fully turbulent flow. These boundary layer solutions must be calculated via the exact equations presented in chapter 2, or else they must be approximated for by following a relevant boundary layer analysis (e.g. George and Capp, 1979).

The $k - \epsilon$ model as set out in sub-section 3.2 would not be expected to be applicable to our particular problem. It generally only satisfies the first of the constraints above. There would be no generation of Reynolds stresses and it would be difficult or impossible for such a scheme to model the diffusive properties of our problem. However, the rather major modifications of section 4.1 ought to make its use more satisfactory, with the Reynolds stresses being the only terms not conveniently modelled.

The full Reynolds stress model of section 3.4 ought to fair a little better. This time it satisfies constraints (i) and (ii), since this closure contains equations in the transport of the Reynolds stresses and the scalar heat flux and the buoyancy is nearly always included in this model. However, the boundary layer equations or wall functions would still be inapplicable in most codes. A commercial package would therefore have to have a facility whereby one could provide one's own equations for the boundary layer. A final comment on this point should be made. The flows with which we are concerned involve a Rayleigh-Taylor type instability along the top surface. The boundary conditions and corresponding boundary layer behaviour along this top surface are a complete unknown in turbulent flows.

Throughout this report, we have mentioned only the basic physical properties which a model should posses. No mention has been made of the more complicated physics expected in strongly-convective flows. (e.g. wall reflection, streamline curvature etc.). Based upon the problems experienced by researchers working upon shear-driven turbulence in complicated flows, one must assume that the lower level schemes (e.g. $k - \epsilon$ or ASM) would have difficulty in modelling the flow accurately. One would expect answers, as we have indicated in this report, but whether such answers will be realistic is another matter. These comments may not apply to the full Reynolds stress closure and this should probably be the recommended starting point when modelling flows of the type which we have considered in this report (Launder, 1989; Rodi, 1989).

Without the comparison of numerical solutions with experimental data, we cannot comment further regarding the application of mean-shear driven turbulence models to convective flows. We conclude, therefore, by suggesting that a great deal more work needs to be done with regard to the problem of highly convective flows. Experiments must be conducted which can provide data with which to compare numerical codes. The experiments must be able to reach Rayleigh numbers of at least 10^9 in order to represent fully-turbulent flow and the geometry and the material must be relevant to the flows of this report. The codes must be updated so that they represent more closely a turbulent flow which is driven by convection. In particular, the boundary layer for a vertical surface must compare with that presented in George and Capp (1979). Finally, the structure of the top boundary must be investigated analytically and reasonable approximations must be found so that a complete turbulence model for these flows is specified.

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