UNIVERSITY OF CALIFORNIA Los Angeles

Numerical Simulation of Tropical Cumulus Clouds and their Interaction with the Subcloud Layer

A dissertation submitted in partial satisfaction of the requirements for the degree Doctor of Philosophy in Atmospheric Sciences

by

Steven Keith Krueger

Appendix A

THIRD-ORDER ENSEMBLE MEAN TURBULENCE CLOSURE MODEL

A.1 ENSEMBLE MEAN CLOSURE

Ensemble mean turbulence closure models predict ensemble means. An ensemble mean is a quantity's value at a point in space and time averaged over infinitely many flow realizations. These realizations differ only infinitesimally in their initial conditions. Due to subsequent development of flow instabilities, the realizations will visibly differ after a short time. The ensemble mean thus includes the averaged effect of the instabilities upon the flow.

One realization can suffice to determine the ensemble mean in homogeneous flows. Homogeniety exists when a running average--taken over a 'region' larger than the fluctuation scale but smaller than the flow domain--does not vary. Such a 'region' can be a length, an area, a volume, or a time interval, as well as a space-time area or volume. The average over a 'region' is then the ensemble mean. For example, the ensemble mean of a horizontally homogeneous flow is the flow's horizontal average.

Atmospheric flows are never truly homogeneous. However, due to the scale separation between turbulence and larger-scale circulations, local homogeniety usually exists. This means that our running average varies, but relatively slowly and on scales characteristic of the larger-scale flow. For example, a wind speed trace from a coastal station will show turbulent fluctuations as well as diurnal variations due to the sea breeze. To get ensemble mean wind speeds, we should choose an averaging 'region' to preserve the diurnal variations, but eliminate the turbulent ones. If the turbulent time scale is 100 seconds, we should use an averaging interval of about 1000 seconds, or 15 minutes.

By using Reynolds decomposition, we can form a set of equations that describes the evolution of the ensemble mean fields. We divide each field into its ensemble mean and its departure. For example, consider the governing equations for a homogenous, incompressible fluid at high Reynolds number:

$$\frac{\partial \widetilde{\mathcal{U}}_{i}}{\partial t} + \widetilde{\mathcal{U}}_{i,j} \widetilde{\mathcal{U}}_{j} = -\frac{1}{f} \widetilde{\beta}_{,i}$$

(A.1)

$$\widetilde{\mathcal{U}}_{i,i} = 0$$
.

In this appendix, we use Cartesian tensor notation. Hereafter, we will use "kinematic" pressure, p/ρ .

Decompose the variables into the ensemble mean and the departure:

$$\widetilde{\mathcal{U}}_{i} = \mathcal{U}_{i} + u_{i},
\widetilde{p} = P + p.$$

Substitute these into (A.1) and average to get the ensemble mean governing equations:

$$\frac{\partial \Box i}{\partial t} + \Box i, j \Box j + (\overline{u_i u_j}), j = -P, i,$$

$$\Box i, i = Q,$$
(A.2)

where the overbar indicates an ensemble mean. We now have more unknowns than equations. To close (A.2) we need to specify the Reynolds stress tensor $\overline{\mathcal{U}_i\mathcal{U}_j}$. This is the problem of ensemble mean closure.

The simplest type of closure assumes that the stress tensor (in this example) is completely determined by the current mean velocity field. This is called *first-order closure*, or more properly, *first-moment closure*. Second-order closure assumes that the past history of the stress tensor also matters, so we use a tendency equation. The additional unknowns introduced by this equation are modeled in terms of mean and second-moment quantities. These unknowns include third moments. If the third moments are instead determined from tendency equations, we have third-order closure. Fig. A.1 schematically shows the various closure types.

A.2 FIRST-ORDER CLOSURE MODELS (K-MODELS)

The first-order or "eddy viscosity" model for the Reynolds stress tensor is

$$\overline{\mathcal{U}_{i}\mathcal{U}_{j}} = \frac{1}{3} \delta_{ij} \overline{\mathcal{U}_{k}\mathcal{U}_{k}} - K\left(\mathcal{U}_{i,j} + \mathcal{U}_{j,i}\right). \tag{A.3}$$

This is the simplest relationship that satisfies tensor invariance and the continuity equation. K, the eddy viscosity, is of the order ql, where q and l are the velocity and length scales of the energy-containing eddies (those responsible for turbulent transport). Thus, K is a property of the flow, not the fluid.

CLOSURE MODELS

First-order closure model :

$$\left\{ \frac{u_{i}u_{j}}{u_{i}\theta} \right\}$$

Second-order closure model:

$$\left\{ \frac{\overline{u_i u_j}}{\overline{u_i \theta}} \right\}$$

Third-order closure model:

$$\left\{ \begin{array}{c} \frac{\overline{u_{i}u_{j}u_{k}u_{l}}}{\overline{u_{i}u_{j}^{\prime}}_{k}^{\prime}} \\ \text{etc.} \end{array} \right\} \quad \stackrel{\bullet}{\rightarrow} \quad \text{diagnostically} \quad \left\{ \begin{array}{c} \overline{u_{i}u_{j}}\\ \overline{u_{i}^{\prime}}\\ \overline{u_{i}^{\prime}}_{k}^{\prime}\\ \overline{u_{i}^{\prime}}_{k}^{\prime}\\ \overline{u_{i}^{\prime}}_{k}^{\prime}\\ \overline{u_{i}^{\prime}}_{k}^{\prime}\\ \overline{u_{i}^{\prime}}_{k}^{\prime}\\ \overline{u_{i}^{\prime}}_{k}^{\prime}\\ \overline{u_{i}^{\prime}}_{k}^{\prime}\\ \overline{u_{i}^{\prime}}_{k}^{\prime}\\ \overline{u_{i}^{\prime}}_{k}^{\prime}\\ \end{array} \right\} \quad \stackrel{\bullet}{\rightarrow} \quad \text{prognostically} \quad \left\{ \begin{array}{c} \overline{u_{i}u_{j}}\\ \overline{u_{i}^{\prime}}\\ \overline{u_{i}^{\prime}}_{k}\\ \overline{u_{i}^{\prime}}_{k}\\ \overline{u_{i}^{\prime}}_{k}^{\prime}\\ \end{array} \right\} \quad \stackrel{\bullet}{\rightarrow} \quad \text{prognostically} \quad \left\{ \begin{array}{c} \overline{u_{i}u_{j}}\\ \overline{u_{i}^{\prime}}\\ \overline{u_{i}^{\prime}}\\ \overline{u_{i}^{\prime}}\\ \overline{u_{i}^{\prime}}\\ \overline{u_{i}^{\prime}}\\ \end{array} \right\} \quad \stackrel{\bullet}{\rightarrow} \quad \text{prognostically} \quad \left\{ \begin{array}{c} \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}^{\prime}}\\ \overline{u_{i}^{\prime}}\\ \overline{u_{i}^{\prime}}\\ \end{array} \right\} \quad \stackrel{\bullet}{\rightarrow} \quad \text{prognostically} \quad \left\{ \begin{array}{c} \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}^{\prime}}\\ \overline{u_{i}^{\prime}}\\ \end{array} \right\} \quad \stackrel{\bullet}{\rightarrow} \quad \text{prognostically} \quad \left\{ \begin{array}{c} \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}^{\prime}}\\ \overline{u_{i}^{\prime}}\\ \end{array} \right\} \quad \stackrel{\bullet}{\rightarrow} \quad \text{prognostically} \quad \left\{ \begin{array}{c} \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}^{\prime}}\\ \overline{u_{i}u_{j}^{\prime}}\\ \end{array} \right\} \quad \stackrel{\bullet}{\rightarrow} \quad \left\{ \begin{array}{c} \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}u_{k}}\\ \end{array} \right\} \quad \stackrel{\bullet}{\rightarrow} \quad \left\{ \begin{array}{c} \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}u_{k}}\\ \overline{u_{i}u_{j}u_{k}}\\ \end{array} \right\} \quad \stackrel{\bullet}{\rightarrow} \quad \left\{ \begin{array}{c} \overline{u_{i}u_{k}u_{k}}\\ \overline{u_{i}u_{k}u_{k}}\\ \overline{u_{i}u_{k}u_{k}}\\ \overline{u_{i}u_{k}}\\ \overline{u_{i}u_{k}u_{k}}\\ \overline{u_{i}u_{k}}\\ \overline{u_{i}u_{k}u_{k}}\\ \overline{u_{i}u_{k}}\\ \overline{u_{i}u_{k$$

$$\left\{
\begin{array}{l}
\overline{u_i u_j} \\
\overline{u_i \theta} \\
\overline{\theta^2} \\
\overline{u_i u_j \theta} \\
\overline{u_i \theta^2} \\
\overline{u_i \theta^3}
\end{array}
\right\}$$

Figure A.1

First-order closure is a limiting case of the more general secondorder closure. First-order closure is a good approximation only when dissipation and shear production dominate the turbulence energy budget; it is not a good approximation for flows with significant transport or buoyant generation of turbulence energy. Because these effects are often present in the ABL, there is motivation to use second- or third-order closure for ABL modeling.

A.3 SECOND-ORDER CLOSURE MODELS

To generate differential equations for Reynolds stress, heat flux, and other turbulence moments, we use Reynolds decomposition. We cannot solve the resulting second-moment equations exactly because they contain unknown third-moments. Many closure approximations for these equations have been proposed over the past twenty years. Less expensive computer time has now made simplified second-moment models a practical alternative to eddy diffusivity models.

We shall first derive and interpret the equations governing the evolution of the stress tensor $\overline{\mathcal{U}_i\,\mathcal{U}_k}$ and the temperature flux vector $\overline{\mathcal{U}_i\,\theta}$. Starting with the stress tensor, we note that

$$\frac{\partial}{\partial t} \frac{u_i u_k}{u_i u_k} = u_i \frac{\partial u_k}{\partial t} + u_k \frac{\partial u_i}{\partial t}.$$

Thus we multiply the u_k -equation by u_i , average, and add this to the equation with i and k interchanged. The result is

$$\frac{\partial}{\partial t} \overline{u_{i}u_{k}} = -U_{i,j} \overline{u_{j}u_{k}} - U_{k,j} \overline{u_{j}u_{i}} - (\overline{u_{i}u_{k}} U_{j}), j$$

$$- (\overline{u_{i}u_{j}u_{k}}),_{j} - (\overline{u_{k}p},_{i} + \overline{u_{i}p},_{k})$$

$$+ \frac{g_{i}}{T} \overline{u_{k}\theta_{v}} + \frac{g_{k}}{T} \overline{u_{i}\theta_{v}} + \nu \overline{u_{k,jj}u_{i}} + \nu \overline{u_{i,jj}u_{k}}.$$
(A.4)

Let's identify the terms on the right side of (A.4). The first two, representing products of turbulent stress and mean shear, are called shear production terms; they are normally sources of $\overline{\mathcal{U}_i\,\mathcal{U}_k}$. The third and fourth are divergences of the mean and turbulent fluxes of $\overline{\mathcal{U}_i\,\mathcal{U}_k}$; we call these advection and transport, respectivley. They integrate to zero over the flow volume by the divergence theorem, and hence represent the movement of $\overline{\mathcal{U}_i\,\mathcal{U}_k}$ from one part of the flow to another. The fifth term is a covariance of fluctuating pressure and velocity. The sixth and seventh are buoyancy terms, and the final pair represent viscous effects.

The same procedure gives a temperature flux equation:

$$\frac{\partial}{\partial t} \overline{\theta u_{i}} = -U_{i,j} \overline{\theta u_{j}} - \Theta_{,j} \overline{u_{i}u_{j}} - (\overline{\theta u_{i}} U_{j}),_{j}$$

$$- (\overline{\theta u_{i}u_{j}}),_{j} - \overline{p_{,i}\theta} + \frac{g_{i}}{T} \overline{\theta_{v}\theta}$$

$$+ v \overline{u_{i,jj}\theta} + \alpha \overline{\theta_{,jj}u_{i}}.$$
(A.5)

The same types of terms that appeared in (A.4) also appear here.

The production, advection and buoyancy terms in (A.4) and (A.5) involve covariances of the turbulence field as well as the mean values U and Θ . These terms can be considered known if the model set contains equations for each covariance and for U and Θ . However, the remaining terms--molecular, pressure covariances, and transport--are not directly related to the covariances or the mean fields, and must at this point be regarded as unknowns. This is the closure problem in the second-moment approach: specifying these unknown terms so the set can be solved.

A.4 THE CLOSURE PROBLEM

I cannot give a comprehensive review here of second-order modeling. Instead, I will briefly describe a well-known second-moment model, the Mellor-Yamada model (Mellor, 1973).

Let's look again at the second-moment equations we just derived, (A.4) and (A.5). We can separate the pressure covariance terms in (A.4) into a pressure transport term

and a pressure redistribution term

$$p\left(U_{i,k} + U_{k,i}\right)$$
.

Similarly, we can write the pressure covariance term in (5) as

$$-(\overline{p\theta})_{,i} + \overline{p\theta_{,i}}$$
.

We also rewrite the molecular terms in (A.4) as

$$v \overline{u_{i,jj}u_k} + v \overline{u_{k,jj}u_i} = v (\overline{u_iu_k}),_{jj} - 2 v \overline{u_{i,j}u_{k,j}}.$$

The first term on the right is the molecular diffusion, which is negligible compared to turbulent transport, and the second is the dissipation. Similarly, we write the molecular terms in (A.5) as

$$v \overline{u_{i,jj}\theta} = v(\theta u_i),_{jj} - v(\overline{\theta, u_i}),_{j} - v \overline{u_{i,j}\theta,_{j}},$$

$$\alpha \ \overline{\theta_{,jj}u_{i}} = \alpha \ (\overline{\theta u_{i}})_{,jj} - \alpha \left(\theta \ \mathcal{U}i,j\right)_{,j} - \alpha \ \overline{\theta_{,j}u_{i,j}} \ .$$

Only the extreme right terms are retained in high Reynolds number flows.

The temperature variance $\overline{\theta^2}$ appears in (A.5). We can derive a differential equation for it as we did for $\overline{\mathcal{U}_i\mathcal{U}_k}$ and $\overline{\mathcal{U}_i\mathcal{Q}}$.

Substituting for the pressure covariance and molecular terms in (A.4), (A.5), and the $\overline{\theta^2}$ equation, we obtain the equations shown below. The underlined terms must be modeled.

$$\frac{\partial u_{i}u_{j}}{\partial t} + \frac{\partial}{\partial x_{k}} \left[U_{k}u_{i}u_{j} + u_{k}u_{i}u_{j} - \nu \frac{\partial}{\partial x_{k}} u_{i}u_{j} \right] + \frac{\partial}{\partial x_{j}} \frac{\partial}{\partial x_{i}} + \frac{\partial}{\partial x_{j}} \frac{\partial}{\partial x_{i}} = -\frac{\partial}{\partial x_{i}} \frac{\partial U_{j}}{\partial x_{k}} - \frac{\partial}{\partial x_{k}} \frac{\partial}{\partial x_{k}} \frac{\partial}{\partial x_{k}} - \beta(g_{j}u_{i}\theta + g_{i}u_{j}\theta) + \frac{\partial}{\partial x_{i}} \frac{\partial}{\partial x_{k}} \frac{\partial}{\partial x_{k}}$$

$$\frac{\partial \overline{u_{j}\theta}}{\partial t} + \frac{\partial}{\partial x_{k}} \left[U_{k}\overline{\theta u_{j}} + \overline{u_{k}u_{j}\theta} - \alpha u_{j} \frac{\partial \overline{\theta}}{\partial x_{k}} - \nu \frac{\partial u_{j}}{\partial x_{k}} \right] \\
+ \frac{\partial}{\partial x_{j}} \overline{p\theta} \\
= -\overline{u_{j}u_{k}} \frac{\partial \Theta}{\partial x_{k}} - \overline{\theta u_{k}} \frac{\partial U_{j}}{\partial x_{k}} - \beta g_{j}\overline{\theta^{2}} + \overline{p} \frac{\partial \overline{\theta}}{\partial x_{j}} \\
- (\alpha + \nu) \frac{\partial u_{j}}{\partial x_{k}} \frac{\partial \overline{\theta}}{\partial k_{k}},$$

$$\frac{\partial \overline{\theta^2}}{\partial t} + \frac{\partial}{\partial x_k} \left[U_k \overline{\theta^2} + \overline{u_k \theta^2} - \alpha \frac{\partial \overline{\theta^2}}{\partial x_k} \right] \\
= -2\overline{u_k \theta} \frac{\partial \Theta}{\partial x_k} - 2\alpha \frac{\partial \overline{\theta}}{\partial x_k} \frac{\partial \Theta}{\partial x_k}$$

A.5 THE MELLOR-YAMADA SECOND-ORDER CLOSURE MODEL

The Mellor-Yamada model was one of the first second-order models. It is based on our knowledge of simple turbulent flows and the requirement of tensor invariance. The modeled terms have the same tensor properties as the original terms, and their coefficients are determined from neutral flow measurements. Since the Mellor-Yamada model was introduced, more accurate ways to model turbulent transport in the convective PBL have been developed (Andre et al. 1978; Lumley, Zeman and Seiss, 1978) but at a considerable computational cost.

The transport terms are modeled as down-gradient diffusion terms. The proportionalty constant is like an eddy viscosity coefficient so Mellor and Yamada use $q\lambda$, where q is the turbulent velocity scale (the square root of twice the turbulent kinetic energy) and λ is a turbulent length scale.

The pressure redistribution term redistributes turbulence kinetic energy among components and destroys off-diagonal stresses. It is modeled as a tendency toward isotropy:

$$-\frac{g}{3l_1}\left(\overline{U_iU_k}-\delta ik\frac{g^2}{3}\right)+C_1 q^2\left(U_{i,k}+U_{k,i}\right).$$

The model for this term also includes a *rapid term* proportional to the mean deformation.

Mellor and Yamada neglect the pressure transport terms since little is known about them and measurements show that they are usually small.

The model for the molecular dissipation is independent of the viscosity. The dissipation rate is approximately the rate of energy transfer from large eddies to smaller eddies; thus it is modeled as

$$\frac{g^3}{\Lambda_1}$$

where Λ_1 is a length scale for the large eddies. Also the small-scale turbulence is assumed to be isotropic so that the dissipation is equally divided among the turbulent energy components. The table on the next page summarizes the modeling assumptions.

Each modeled term introduces a length scale. We assume these are proportional to a master length scale. Specifying this length scale is the remaining closure problem. Blackadar (1962) proposed

$$\ell = \frac{kz}{1 + kz/l\omega}$$

$$\frac{1}{p\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)} = -\frac{q}{3l_1}\left(\frac{\partial u_i}{\partial u_j} - \frac{\delta_{ij}}{3}q^2\right) + Cq^2\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)$$

$$\overline{p\frac{\partial \theta}{\partial x_j}} = -\frac{q}{3l_2}\overline{u_j\theta}$$

$$\overline{pu_i} = \overline{p\theta} = 0$$

$$2\nu \frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k} = \frac{2}{3} \frac{q^3}{\Lambda_1} \delta_{ij}$$

$$(\alpha + \nu) \frac{\partial u_j}{\partial x_k} \frac{\partial \theta}{\partial x_k} = 0$$

$$2\alpha \frac{\overline{\partial \theta} \overline{\partial \theta}}{\partial x_k} \frac{\partial \theta}{\partial x_k} = 2\frac{q}{\Lambda_2} \overline{\theta^2}$$

$$\overline{u_k u_i u_j} = -q \lambda_1 \left(\frac{\partial \overline{u_i u_j}}{\partial x_k} + \frac{\partial \overline{u_i u_k}}{\partial x_j} + \frac{\partial \overline{u_i u_k}}{\partial x_i} \right)$$

$$\overline{u_k u_j \theta} = -q \lambda_2 \left(\frac{\partial \overline{u_k \theta}}{\partial x_j} + \frac{\partial \overline{u_j \theta}}{\partial x_k} \right)$$

$$\overline{u_k \theta^2} = -q \lambda_3 \frac{\partial \theta^2}{\partial x_k}$$

Table A.1

for use in atmosperic boundary layers. k is von Karman's constant, and $\mathcal{L}_{\boldsymbol{\omega}}$ is a length, which modelers usually prescribe, but may instead determine from a formula such as

$$\ell_{\infty} = \propto \frac{\int_{0}^{\infty} q \, z \, dz}{\int_{0}^{\infty} q \, dz}$$

where $\alpha=0.1$ is usually used.

A.6 THIRD-ORDER CLOSURE MODELS

Second-order closure models like Mellor and Yamada's underpredict the growth of the convective PBL (Yamada and Mellor, 1975). They don't transport enough turbulence to the PBL top to support active entrainment, so the PBL deepens too slowly. Third-order closure models--which use approximate conservation equations for the third moments-- predict realistic growth rates (Andre et al., 1978). The models include the effects of buoyancy on turbulent transport.

Both second- and third-moment closure models have been used to simulate the evolution of a convective boundary layer. The convective atmospheric boundary layer measured on day 33 of the Wangara experiment was simulated by Yamada and Mellor (1975) (YM) and by Andre et al., (1978) (A). Fig. A.2 shows the simulated

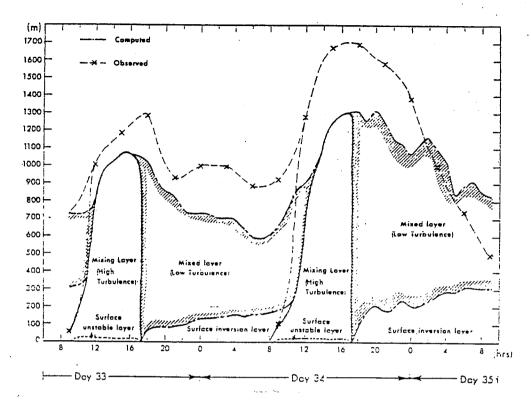


Figure A.2

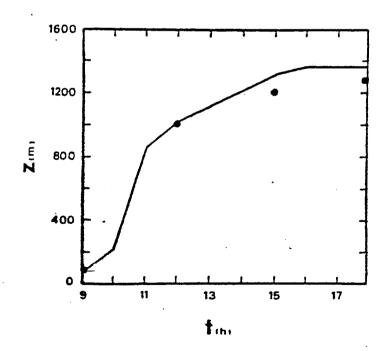
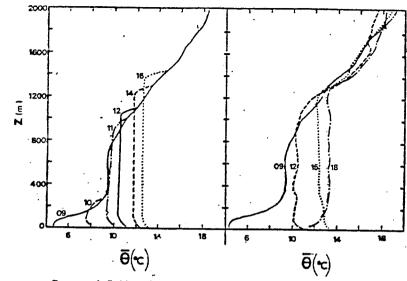


Figure A.3



Computed (left) and observed (right) profiles of mean virtual potential temperature during Day 33.

Figure A.4

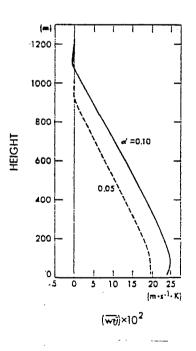


Figure A.5

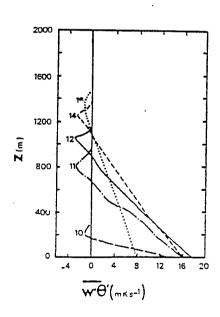
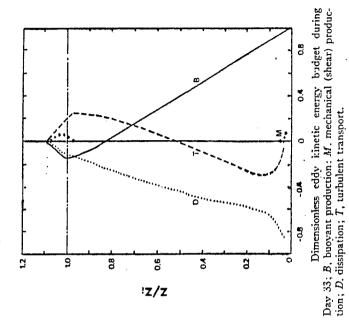


Figure A.6





Computed profiles of the terms in the turbulent kinetic energy equation (12), units m² s⁻², at 1400 on Day 34.

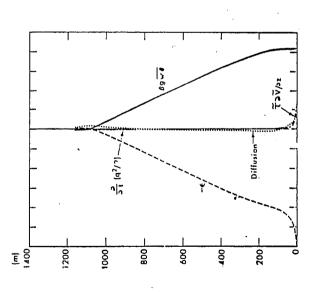


Figure A.7

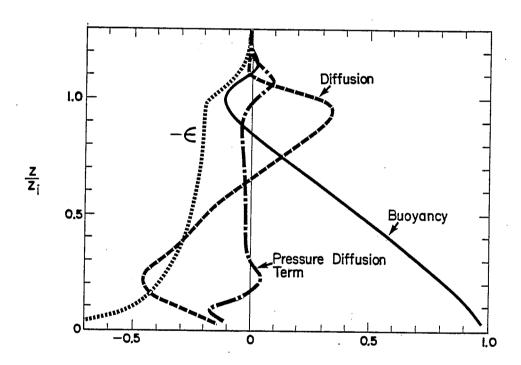


Figure A.9

evolution of the mixed layer depth using a second-moment model (YM) and Fig. A.3 shows the same using a third-moment model (A). Each figure also shows the observed depth. YM underpredicts the growth of the daytime mixed layer, while A nearly matches the observed depths. (The mixed layer depth is the height of the minimum value of $\widehat{w\theta}$.)

Fig. A.4 shows how the mixed layer grows: potentially warm overlying air is entrained at the mixed layer top. This process consumes turbulent kinetic energy (TKE), as indicated by the negative we in the entrainment region. Figs. A.5 and A.6 show we simulated by YM and A, respectively. Entrainment must be more active in A since we is more negative.

The simulated TKE budgets clearly show the difference between the two models. Fig. A.7 shows that turbulent transport of TKE is unimportant throughout the mixed layer in YM. Since the only possible sources of TKE at the mixed layer top are turbulent transport and mechanical (shear) production, and both are unimportant in this simulation, there cannot be active entrainment. Fig. A.8 shows the TKE budget for A, the third-moment closure simulation. In this case, turbulent transport is a significant source of TKE at the mixed layer top.

There are no turbulence measurements from the Wangara simulation to compare with, but we do have data from a large-eddy simulation

(Deardorff, 1974), Fig. A.¶.. These data are nearly as reliable as measurements themselves since such simulations depend very little on modeling assumptions. The simulated TKE is very similar to A's, especially for the turbulent transport. I conclude that third-moment closure can accurately simulate a convective boundary layer, but second-moment closure cannot.

Now let's look at the third-moment equation for the turbulent flux of $u_i^{}u_i^{}$ to see how buoyancy affects it.

The conservation equation for $\overline{\mathcal{U}_i\mathcal{U}_k\mathcal{U}_j}$, the turbulent flux in the $\overline{\mathcal{U}_i\mathcal{U}_k}$ -equation, is

$$\frac{\partial}{\partial t} \overline{u_{i}u_{k}u_{j}} = -\left[U_{i,m} \overline{u_{m}u_{j}u_{k}} + \dots\right]$$

$$-\left(\overline{u_{i}u_{m}u_{j}u_{k}}\right),_{m}$$

$$+\left[\left(\overline{u_{i}u_{m}}\right),_{m} \overline{u_{j}u_{k}} + \dots\right]$$

$$-\left[\overline{p_{i}u_{j}u_{k}} + \dots\right]$$

$$+\left[\frac{g_{i}}{T} \overline{\theta_{v}u_{j}u_{k}} + \dots\right]$$

$$-2v\left[\overline{u_{i,j}u_{j,j}u_{k}} + \dots\right].$$

$$(A.6)$$

The $+\dots$ indicates two more terms obtained from the first by cyclic permutation of the indices i, j, k. The terms in (A.b) are, in

order, shear production, turbulent transport, turbulent production, pressure interaction, buoyancy, and molecular. The turbulent transport term here is a fourth moment. Even-order moments of velocity and temperature (but *not* derivative moments) are usually Gaussian, to a good approximation. If we use a Gaussian model for this fourth moment, we can write

$$\frac{\overline{u_i u_i u_j u_k}}{i_i m_j i_k} \simeq \frac{\overline{u_i u_i}}{u_j u_k} + \frac{\overline{u_i u_j}}{u_i i_j} \frac{\overline{u_i u_k}}{m_k} + \frac{\overline{u_i u_k}}{u_i i_k} \frac{\overline{u_i u_j}}{m_j}. \tag{A.7}$$

This allows us to combine transport and turbulent production in (A.6) to get

$$- (\overline{u_{\underline{i}}^{\underline{u}}_{\underline{m}}^{\underline{u}}_{\underline{j}}^{\underline{u}}_{\underline{k}}}),_{\underline{m}} + [(\overline{u_{\underline{i}}^{\underline{u}}_{\underline{m}}}),_{\underline{m}} \overline{u_{\underline{j}}^{\underline{u}}_{\underline{k}}} + ..]$$

$$\simeq [-(\overline{u_{\underline{j}}^{\underline{u}}_{\underline{k}}}),_{\underline{m}} \overline{u_{\underline{i}}^{\underline{u}}_{\underline{m}}} + ..]. \tag{A.8}$$

Let's consider (A.6) in an idealized, near-neutral surface layer, using the result (A.8) of our Gaussian transport approximation. Assume that the pressure (Pijk) and molecular (Mijk) terms in (A.6) behave roughly like their counterparts in the second-moment equations, so that

$$P_{ijk} + M_{ijk} \simeq -\frac{\overline{u_i u_j u_k}}{\tau}.$$
 (A.9)

With (A.9), the $U:U_h^*U_k$ -equation in this case reduces to

$$-\tau[(\overline{u_{j}u_{k}}),_{m}\overline{u_{i}u_{m}} + (\overline{u_{k}u_{i}}),_{m}\overline{u_{j}u_{m}} + (\overline{u_{i}u_{j}}),_{m}\overline{u_{k}u_{m}}] \simeq \overline{u_{i}u_{j}u_{k}}. \quad (A.10)$$

This is exactly the gradient-diffusion approximation used for in many models. Mellor and Yamada further assumed that

and used

$$Z = \frac{\mathcal{L}}{g}$$

to obtain their gradient-diffusion model.

In the very unstable surface layer, or in the mixed layer during even mildly unstable conditions, the buoyant term in (A.6) will be important. Then (A.6) becomes

$$\overline{u_{i}u_{j}u_{k}} = -\tau[(\overline{u_{j}u_{k}}),_{m} \overline{u_{i}u_{m}} + (\overline{u_{k}u_{i}}),_{m} \overline{u_{j}u_{m}} + (\overline{u_{i}u_{j}}),_{m} \overline{u_{k}u_{m}}]$$

$$+ \tau[\frac{g_{i}}{T} \overline{\theta_{v_{j}u_{k}}} + \frac{g_{j}}{T} \overline{\theta_{v_{i}u_{k}}} + \frac{g_{k}}{T} \overline{\theta_{v_{i}u_{j}}}].$$
(A.11)

Now the gradient-diffusion model (A.10) for $\overline{\mathcal{U}_i\mathcal{U}_j\mathcal{U}_k}$ need not hold. If the buoyant term in (A.11) is also important, $\overline{\mathcal{U}_i\mathcal{U}_j\mathcal{U}_k}$ can depend on more than second-moment gradients.

Consider the situation for $\overline{W^3}$ in the unstable surface layer. Both $\overline{W^3}$ and $\partial \overline{W^2}/\partial Z$ are observed to be positive there, while (A.10) implies

$$\overline{w^3} = -3\tau w^2 \frac{1}{\partial w^2} / \partial z$$

or that they have opposite sign. Thus the usual gradient-diffusion model fails. One reason for this failure is that the buoyant term in the $\overline{W^3}$ budget (A.6) is significant in the unstable surface layer.

Strong buoyancy effects are the rule in the PBL. Thus we should expect that gradient-diffusion approximations (such as (A-IO)) for third moments will not be accurate.

A.7 A THIRD-MOMENT TURBULENCE MODEL

I am using a third-moment closure model in the cumulus ensemble model. This is necessary not only to model the subcloud layer turbulence as accurately as possible without going to the expense of a large-eddy model, but also to model the turbulence in the clouds in a realistic manner. In the lower cloud layer, turbulent-scale condensation is important due to many shallow cumulus clouds. These clouds do not always have organized "cloud-scale" motions. Their kinetic energy is mostly on the turbulent scales. To accurately include the turbulent effects of these clouds, a turbulence model which is realistic in convective boundary layers is required.

Even though the cloud-scale motions are governed by the anelastic equations, we assume that turbulent-scale motions are governed by the Boussinesq (or shallow anelastic) equations. This is valid as long as the turbulent motions are shallow compared the scale height of the atmosphere.

The turbulence model chosen is essentially that developed by Andre et al. (1976a; 1978) and used by Bougeault (1981b). It is

Table A.2 Closure assumptions for two turbulence models.

| Term | Andre | Mellor-Yamada |
|--------------------------|---|---|
| pressure- correlation | Return-to-isotropy and rapid terms (mean shear, buoyancy). | Neglects some rapid terms. |
| turbulent trańsport | Approximate rate eqs. (quasi-Guassian, eddy-damped approxima- tion) used. Buoyancy effects included. Clipping approximation to enforce realizability. | Down-gradient model appropriate to nearly isotropic neutal shear flow. No buoyancy effects. |
| pressure transport | -1/5 * energy transport. | Neglected. |
| molecular terms | Isotropic. Inviscid estimate dissipation rate. Turbulent must be specifed. Destruct variances proportional to di | length scale |

more physically based than the Mellor-Yamada model. Table A.2 presents a comparison.

In the model I am using, the closure assumptions for the pressure correlations, as well as for the third-moments, differ from those of Mellor-Yamada (MY). The pressure correlations are modeled as the sum of a pressure transport term, a return-to-isotropy term, and a rapid term. The pressure transport slightly reduces turbulent kinetic energy transport. The return-to-isotropy term is standard, and the rapid terms (which MY took proportional to the mean deformation) are modeled following Launder (1975).

The third-moment equations present new closure problems. They introduce unknown pressure correlations, molecular terms and fourth moments. The latter are expressed in terms of second moments using the quasi-Gaussian approximation:

$$\overline{abcd} = \overline{ab} \, \overline{cd} + \overline{ac} \, \overline{bd} + \overline{ad} \, \overline{bc}$$
.

Pressure correlations are assumed to follow closures like the second-moment pressure correlations. However, I do not include rapid terms. Molecular terms are neglected except in scalar correlation equations, for which there are no pressure correlation terms. The "clipping" approximation (Andre et al., (1976a) is used to limit the growth of the third-moments. For a correlation $\overline{\alpha\beta\chi}$, the clipping approximation is to enforce

$$|\overline{\alpha\beta\gamma}| \leqslant \min \begin{bmatrix} \overline{\alpha^{2}(\overline{\beta^{2}} \overline{\gamma^{2}} + \overline{\beta} \overline{\gamma^{2}})} \end{bmatrix}^{\frac{1}{2}} \\ \overline{\beta^{2}(\overline{\alpha^{2}} \overline{\gamma^{2}} + \overline{\alpha} \overline{\gamma^{2}})} \end{bmatrix}^{\frac{1}{2}} \\ \overline{[\overline{\gamma^{2}(\overline{\alpha^{2}} \overline{\beta^{2}} + \overline{\alpha} \overline{\beta^{2}})}]^{\frac{1}{2}}} \end{bmatrix}.$$

Lumley (1978) theoretically derived a closure model for the third-moment equations that has no more empirical constants than does second-moment closure. I am using his closure constants for the third moment equations.

Since the only widely known and applied third-moment model is the one developed by Andre et al., (1976a; 1978) and extended by Bougeault (1981a,b), I will first point out the differences between my model and Bougeault's, before presenting the model equations I use. My equations differ in only two modeling assumptions. First, I neglect the mean shear production terms in the third moment equations, which Bougeault does not. I neglect these terms because they are not important in strongly buoyant conditions (Andre et al., 1976a,b; Lumley, 1978). I also retain the clipping approximation to damp the growth of the third moments whereas Bougeault uses a "rapid" term in the third moment equations. The clipping approximation is useful because one can judge by the frequency of "clipping" how well the third-moment closure model is doing.

In addition, the equations differ because I use a two-dimensional version, include advection terms, and use a different set of closure constants. Table A.3 compares the values I use with Bougeault's values; c_4 - c_7 are from Zeman and Lumley (1976); c_2 is from Launder

Table A.3

| constant | Bougeault (1981b) | present work |
|----------------|----------------------|-----------------|
| C ₂ | 1.3 | 1.25 |
| C. | 4.5 | 1.75 |
| C 5 | 0 | 0.3 |
| C 6 | 4.85 | 3.75 |
| C7 | 0.4 | 0.33 |
| CB | 6.5 | 5,25-9,25 |
| C10 | 3.9 | 3.75 |
| Cll | 0.4 | 0 |

(1975); and c_8 , c_{10} , and c_{11} are based on Lumley (1978). The most significant differences are in the values for c_4 and c_5

The turbulence model equations can be written as follows, using a and b for h or q_W , and, for simplicity, assuming p is a constant. In the following, \overline{e} is the turbulent kinetic energy, ϵ is the dissipation rate, $\tau=\overline{e}/\epsilon$, and $\beta=g/\overline{T}$.

- 1. The prognostic equations for the 6 mean quantities, u, w, θ , $q_{\rm V}$, $q_{\rm c}$, and $q_{\rm r}$ are given in section 3.2.
- 2. The tendencies of the velocity correlations are

$$\frac{d}{dt} \overline{U_i U_j} = -\left(\overline{U_K U_i U_j} - \frac{\overline{U_K U_e U_e}}{15} \delta_{ij}\right)_{j,k}$$

$$-\left(1 - C_5\right) \left\{\overline{U_i U_K} \ \bigcup_{j,k} + \overline{U_j U_k} \ \bigcup_{i,k} \right\}$$

$$-\beta \overline{U_i \Theta_V} \delta_{3j} - \beta \overline{U_j \Theta_V} \delta_{3i}\right\}$$

$$-\frac{2}{3} \mathcal{E} \delta_{ij} - \frac{C_4}{T} \left(\overline{U_i U_j} - \frac{2}{3} \delta_{ij} \overline{\mathcal{E}}\right)$$

$$+ C_5 \frac{2}{3} \delta_{ij} \left\{\beta \overline{W \Theta_V} - \overline{U_e U_K} U_{e,k}\right\}.$$

3. The scalar correlation tendencies are

$$\frac{d}{dt} \overline{ab} = -(\overline{u_k ab})_{,k} - \{\overline{au_k} B_{,k} + \overline{bu_k} A_{,k}\} - \frac{c_2}{\tau} \overline{ab}.$$

4. The scalar flux equations are

$$\frac{d}{dt} \overline{u_i a} = -(\overline{u_k u_i a})_{,k} - \overline{u_i u_k} A_{,k}$$

$$-(1-C_7) \left\{ \overline{u_k a} \bigsqcup_{i,k} -\beta \delta_{3i} \overline{\theta_{v} a} \right\} - \frac{c_6}{7} \overline{u_i a}.$$

5. The equations for the fluxes of velocity correlations are

$$\frac{d}{dt} \overline{u_i u_j u_k} = -\overline{u_i u_k} (\overline{u_j u_k})_{,\ell} - \overline{u_j u_k} (\overline{u_i u_k})_{,\ell}$$

$$-\overline{u_k u_k} (\overline{u_i u_j})_{,\ell} - \frac{c_8}{\tau} (\overline{u_i u_j u_k})$$

$$+ \beta \delta_{3k} \overline{u_i u_j \theta_v} + \beta \delta_{3j} \overline{u_i u_k \theta_v} + \beta \delta_{3i} \overline{u_j u_k \theta_v}.$$

6. The tendencies of the triple scalar correlations are

$$\frac{d}{dt} \overline{a^2b} = -\overline{U_{\ell}b} (\overline{a^2})_{,\ell} - 2 \overline{U_{\ell}a} (\overline{ab})_{,\ell}$$
$$-\overline{U_{\ell}a^2} B_{,\ell} - 2 \overline{U_{\ell}ab} A_{,\ell} - \frac{c_{,o}}{T} \overline{a^2b}.$$

7. For the fluxes of the scalar fluxes, the equations are

$$\frac{d}{dt} \overline{u_i u_j a} = -\overline{u_l a} (\overline{u_i u_j}), \ell - \overline{u_i u_l} (\overline{u_j a}), \ell$$

$$-\overline{u_j u_l} (\overline{u_i a}), \ell - \overline{u_i u_j u_l} A, \ell$$

$$+\beta \overline{u_i a \theta_v} \delta_{3j} +\beta \overline{u_j a \theta_v} \delta_{3i}$$

$$-\overline{u_i u_l a} U_j, \ell - \overline{u_j u_l a} U_i, \ell - \frac{c_8}{\tau} \overline{u_i u_j a}.$$

8. Finally, for the fluxes of scalar correlations, the equations are

$$\frac{d}{dt} \overline{u_i ab} = -\overline{u_i u_\ell} (\overline{ab}), \ell - \overline{u_\ell a} (\overline{u_i b}), \ell$$

$$-\overline{u_\ell b} (\overline{u_i a}), \ell - \overline{u_i u_\ell a} B, \ell - \overline{u_i u_\ell b} A, \ell$$

$$+\beta \overline{\theta_v ab} \delta_{3i} - \frac{c_{\delta}^{s}}{\tau} \overline{u_i ab}.$$

Note that I use different values for c_8 , c_8 , and c_8 , following Lumley (1978).

I found it necessary to include a small diffusion term in in all of the second-moment equations, and both damping term and diffusion terms in all of the third-moment equations. Deardorff (1978) pointed out that diffusion terms are required in the third-moment equations to match analytical solutions of the Gaussian plume.

If F_{ab} and F_{abc} represent the tendencies of \overline{ab} and \overline{abc} given by the model equations above, then the modified equations are

$$\frac{\partial}{\partial t} \overline{ab} = F_{ab} + K_2 \nabla^2 \overline{ab},$$

$$\frac{\partial}{\partial t} \overline{abc} = F_{abc} + K_3 \nabla^2 \overline{abc} - D_3 \overline{abc}$$

where $K_2=K_3=10~\text{m}^2/\text{s}$ and $D_3=0.024~\text{s}^{-1}$ Without these added terms, the model could not simulate the GATE fair-weather boundary layer (see section 3.9).

In the horizontally-homogeneous case, with no mean wind, allowing \overline{uwh} and/or \overline{uwq}_w to be non-zero leads to an instability. (This is a property of the continuous equations.) To guard against this possibility, I enforced $\overline{uwh} = \overline{uwq}_w = 0$ in all of the simulations.

A.8 DISSIPATION RATE AND TURBULENT LENGTH SCALE

I have not had much success with prognostic equations for the dissipation rate in flows which are rapidly evolving, such as in cumulus clouds. Since so little is known about turbulence in cumulus clouds, I chose to use the simpler diagnostic modeling of the dissipation rate. This is known to work well for convective boundary layers (Andre et al., 1976b). As noted in section 3.8, I simulated a cumulonimbus cloud using this formulation for a range of turbulent length scales, and didn't find a strong influence on the cloud dynamics, although it significantly affected the cloud turbulence intensity.

The dissipation rate is calculated from

$$\mathcal{E} = C_1 \frac{\overline{e}^{3/2}}{\int_{1}^{3/2} (2)}$$

where I(z) is calculated from Blackadar's formula (see section A.4), $I_{\infty} = 0.15 \, z_{\text{mix}}$ (Bougeault, 1981b), $z_{\text{mix}} = 400 \, \text{m}$, and $c_1 = 0.14$ (Andre *et al.*, 1978). Above 400 m, I = I(400). There is little guidance for choosing I in the cloud layer.