

The First- and Second-Moment Equations

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16.1 Introduction

A basic goal of fluid dynamics research is to develop a theory to determine statistics of turbulent flows. The most basic statistics are the average values of such variables as the velocity components, the temperature, and the humidity. Additional statistics of interest include second and higher moments of these same fields, singly or in combination. As we will see below, the equations which can be developed to predict the first moments actually involve the second moments, equations to predict the second moments involve the third moments, and so on. This is one of the three closure problems of turbulence. The second closure problem is that equations to predict statistics involving velocity components inevitably involve statistics of the pressure field, which represent additional unknowns. The third closure problem is that the equations for the second (and higher) moments involve important molecular terms, e.g. terms arising from molecular viscosity or molecular conductivity, and these entail statistics of the spatial structure which are also unknown and must be determined through some sort of closure.

16.2 Derivation of the basic equations

16.2.1) Derivation

The anelastic momentum equation can be written in flux form as

$$\frac{\partial u_i}{\partial t} + \frac{1}{\rho_0} \frac{\partial}{\partial x_j} (\rho_0 u_i u_j - \mathfrak{S}_{i,j}) - 2\varepsilon_{i,j,k} u_j \Omega_k = -\frac{\partial}{\partial x_i} \left(\frac{\delta p}{\rho_0} \right) + \frac{\delta \theta}{\theta_0} g_i . \quad (16.1)$$

Here $\delta p = p - p_0$, $\delta \theta \equiv \theta - \theta_0$, and $\mathfrak{S}_{i,j}$ is the viscous stress tensor. The symbol $\varepsilon_{i,j,k}$ denotes 1 if the subscripts run in forward order, -1 if they run in backwards order, and 0 otherwise. We can write $\mathfrak{S}_{i,j}$ as

$$\mathfrak{S}_{i,j} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \delta_{i,j} \left(\mu_B - \frac{2}{3} \mu \right) \frac{\partial u_k}{\partial x_k} , \quad (16.2)$$

where μ is the molecular viscosity, μ_B is the “bulk” viscosity coefficient, which is negligibly small for most gases, and $\delta_{i,j}$ is the Kroneker delta. For air,

$$\mathfrak{S}_{i,j} \cong \mu \frac{\partial u_i}{\partial x_j}. \quad (16.3)$$

The anelastic continuity equation is

$$\frac{\partial}{\partial x_i}(\rho_0 u_i) = 0. \quad (16.4)$$

Using (16.4), we can rewrite the momentum equation in advective form:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial}{\partial x_j} u_i - 2\varepsilon_{i,j,k} u_j \Omega_k - \frac{1}{\rho_0} \frac{\partial}{\partial x_j} \mathfrak{S}_{i,j} = -\frac{\partial}{\partial x_i} \left(\frac{\delta p}{\rho_0} \right) + \frac{\delta \theta}{\theta_0} g_i. \quad (16.5)$$

The *Reynolds decomposition*,

$$(\quad) = \overline{(\quad)} + (\quad)', \quad (16.6)$$

where the overbar denotes an average (see the chapter on Reynolds averaging), allows us to write the continuity equation for the mean flow as

$$\frac{\partial}{\partial x_i}(\rho_0 \bar{u}_i) = 0. \quad (16.7)$$

We can then use (16.6) and (16.7) to write the continuity equation for the fluctuations as

$$\frac{\partial}{\partial x_i}(\rho_0 u'_i) = 0. \quad (16.8)$$

Averaging (16.1) gives us the equation of motion for the mean flow:

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{1}{\rho_0} \frac{\partial}{\partial x_j} (\rho_0 \bar{u}_i \bar{u}_j + \rho_0 \overline{u'_i u'_j} - \overline{\mathfrak{S}_{i,j}}) - 2\varepsilon_{i,j,k} \bar{u}_j \bar{\Omega}_k = -\frac{\partial}{\partial x_i} \left(\frac{\bar{\delta p}}{\rho_0} \right) + \frac{\bar{\delta \theta}}{\theta_0} g_i. \quad (16.9)$$

Here we have used

$$\rho_0 \overline{u_i u_j} = \rho_0 \bar{u}_i \bar{u}_j + \rho_0 \overline{u'_i u'_j}. \quad (16.10)$$

Using the averaged continuity equation, (16.7), Eq. (16.9) can also be written in the

“advective form:”

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} - 2\varepsilon_{i,j,k} \bar{u}_j \Omega_k + \frac{1}{\rho_0} \frac{\partial}{\partial x_j} (-\bar{\mathfrak{T}}_{i,j} + \rho_0 \overline{u'_i u'_j}) = -\frac{\partial}{\partial x_i} \left(\frac{\delta p}{\rho_0} \right) + \frac{\delta \theta}{\theta_0} g_i. \quad (16.11)$$

In (16.9) and (16.11), the new quantity $\rho_0 \overline{u'_i u'_j}$ is called the “*Reynolds stress*,” it appears in parallel with the viscous stress.

Subtracting (16.11) from the advective form of the un-averaged momentum equation, (16.5), and using (16.6), we obtain the momentum equation for the fluctuating part of the wind field:

$$\begin{aligned} \frac{\partial u'_i}{\partial t} + \bar{u}_j \frac{\partial u'_i}{\partial x_j} + u'_j \frac{\partial \bar{u}_i}{\partial x_j} + u'_j \frac{\partial u'_i}{\partial x_j} &= 2\varepsilon_{i,j,k} u'_j \Omega_k - \frac{\partial}{\partial x_i} \left(\frac{\delta p'}{\rho_0} \right) + \frac{\delta \theta'}{\theta_0} g_i \\ &+ \frac{1}{\rho_0} \frac{\partial}{\partial x_j} (\mathfrak{T}'_{i,j} - \rho_0 \overline{u'_i u'_j}) \end{aligned} \quad (16.12)$$

Multiplying (16.12) by $\rho_0 u'_l$ gives

$$\begin{aligned} \rho_0 u'_l \frac{\partial u'_i}{\partial t} + \rho_0 u'_l \bar{u}_j \frac{\partial u'_i}{\partial x_j} + \rho_0 u'_l u'_j \frac{\partial \bar{u}_i}{\partial x_j} + \rho_0 u'_l u'_j \frac{\partial u'_i}{\partial x_j} \\ = 2\varepsilon_{i,j,k} \Omega_k \rho_0 u'_l u'_j - \rho_0 u'_l \frac{\partial}{\partial x_i} \left(\frac{\delta p'}{\rho_0} \right) + \frac{\rho_0 u'_l \delta \theta'}{\theta_0} g_i + u'_l \frac{\partial}{\partial x_j} (\mathfrak{T}'_{i,j} - \rho_0 \overline{u'_i u'_j}). \end{aligned} \quad (16.13)$$

Of course, (16.13) remains valid if i and l are interchanged. Performing this operation, adding the result to (16.13), averaging, and combining terms, we obtain the Reynolds stress equation:

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_0 \overline{u'_i u'_l}) + \frac{\partial}{\partial x_j} (\rho_0 \bar{u}_j \overline{u'_i u'_l} + \rho_0 \overline{u'_i u'_j u'_l} - \overline{u'_i \mathfrak{T}'_{l,j}} - \overline{u'_l \mathfrak{T}'_{i,j}}) = \\ - \rho_0 \overline{u'_l u'_j} \frac{\partial \bar{u}_i}{\partial x_j} - \rho_0 \overline{u'_i u'_j} \frac{\partial \bar{u}_l}{\partial x_j} + 2\varepsilon_{l,j,k} \Omega_k \rho_0 \overline{u'_i u'_j} + 2\varepsilon_{i,j,k} \Omega_k \rho_0 \overline{u'_l u'_j} \\ - \frac{\partial}{\partial x_i} (\overline{u'_l \delta p'}) - \frac{\partial}{\partial x_l} (\overline{u'_i \delta p'}) + \frac{\delta p'}{\rho_0} \frac{\partial}{\partial x_i} (\rho_0 \overline{u'_l}) + \frac{\delta p'}{\rho_0} \frac{\partial}{\partial x_l} (\rho_0 \overline{u'_i}) \\ + \frac{\rho_0}{\theta_0} (\overline{u'_l \delta \theta' g_i} + \overline{u'_i \delta \theta' g_l}) - \left(\overline{\mathfrak{T}'_{i,j} \frac{\partial u'_l}{\partial x_j}} + \overline{\mathfrak{T}'_{l,j} \frac{\partial u'_i}{\partial x_j}} \right). \end{aligned} \quad (16.14)$$

In deriving (16.14), we have made use of (16.7) and (16.8).

We see from (16.14) that the present value of $\overline{\rho_0 u'_i u'_l}$ depends, in general, on its past history. If (16.14) is used to predict $\overline{\rho_0 u'_i u'_l}$, then the result can be used to predict $\overline{u'_i}$, using (16.9). Eq. (16.14) contains the new unknown $\overline{\rho_0 u'_i u'_j u'_l}$ (a “triple correlation,” or “third moment”), however, which must be determined before $\overline{\rho_0 u'_i u'_l}$ can be predicted. In addition, (16.14) contains second moments involving the pressure, and second moments involving the viscous stress tensor. These must also be determined before (16.14) can be used.

A prognostic equation for the triple moment $\overline{\rho_0 u'_i u'_j u'_l}$ can be derived, but this equation contains fourth moments, etc. A possible procedure is to model or parameterize the third moments in terms of the mean flow and the second moments. *This approach is necessarily approximate*, since it involves neglecting the influence of the past history of the third moments. However, much success has been achieved with this approach, which is called “second-order closure.” Further discussion of the third moments is given later.

The rate equation for the Reynolds stress tensor represents nine scalar equations, six of which are independent. The diagonal terms, for which $i = l$, may be written as

$$\begin{aligned} \frac{\partial}{\partial t} \left(\overline{\rho_0 \frac{u'_i u'_i}{2}} \right) + \frac{\partial}{\partial x_j} \left(\overline{\rho_0 u'_j \frac{u'_i u'_i}{2}} + \overline{\rho_0 u'_j \frac{1}{2} u'_i u'_i} - \overline{\mathfrak{T}'_{i,j} u'_i} \right) + \frac{\partial}{\partial x_i} (\overline{\delta p' u'_i}) \\ = 2\varepsilon_{i,j,k} \Omega_k \overline{\rho_0 u'_i u'_j} + \frac{\delta p'}{\rho_0} \frac{\partial}{\partial x_i} (\overline{\rho_0 u'_i}) \\ + \frac{\rho_0}{\theta_0} (\overline{u'_i \delta \theta' g_i}) - \overline{\rho_0 u'_i u'_j} \frac{\partial \overline{u_i}}{\partial x_j} - \overline{\mathfrak{T}'_{i,j}} \frac{\partial \overline{u'_i}}{\partial x_j} . \end{aligned} \quad (16.15)$$

where we temporarily suspend the summation convention for the i subscript only, so that (16.15) represents three equations for the three velocity variances $\overline{\rho_0 \frac{u'_1 u'_1}{2}}$, $\overline{\rho_0 \frac{u'_2 u'_2}{2}}$, and $\overline{\rho_0 \frac{u'_3 u'_3}{2}}$.

The terms on the second line of (16.15) merely redistribute energy among the three individual components, e.g., from $\frac{1}{2} \overline{u'_1 u'_1}$ to $\frac{1}{2} \overline{u'_2 u'_2}$. Of these terms, the one involving pressure is usually the larger, and is typically called the “pressure redistribution” or “return-to-isotropy” term. The rotation term is typically negligible.

The viscous terms on the left-hand side of (16.15) represent transports or spatial redistributions by the viscous force; they do not act as net sources or sinks. In contrast, the viscous terms on the right-hand side of (16.15) represent net sinks of the velocity variances; this can be seen by use of (16.3). These are called “*dissipation*” terms.

Now, reinstituting the summation convention, we “contract” (16.15) to obtain the *turbulence kinetic energy (TKE) equation*:

$$\begin{aligned} \frac{\partial}{\partial t} \left(\rho_0 \frac{\overline{u'^2}}{2} \right) + \frac{\partial}{\partial x_j} \left(\rho_0 \overline{u_j' \frac{u'^2}{2}} + \rho_0 \overline{u_j' \frac{u'^2}{2}} + \overline{\delta p' u_j'} - \overline{u_i' \mathfrak{S}_{i,j}'} \right) = \\ - \rho_0 \overline{u_i' u_j' \frac{\partial u_i}{\partial x_j}} + \frac{\rho_0}{\theta_0} \overline{u_i' \delta \theta' g_i} - \overline{\mathfrak{S}_{i,j}' \frac{\partial u_i'}{\partial x_j}} . \end{aligned} \quad (16.16)$$

The rotation and pressure redistribution terms have cancelled, as expected.

The terms in $\frac{\partial}{\partial x_j} ()$ on the left-hand side of (16.16) represent energy fluxes due to triple moments, pressure-velocity correlations, and viscous stresses. The remaining terms represent mechanical production, buoyant production, and viscous dissipation, respectively. The dissipation term is always a sink of TKE. This can be seen by using (16.3) to write

$$\overline{\mathfrak{S}_{i,j}' \frac{\partial u_i'}{\partial x_j}} = \mu \overline{\left(\frac{\partial u_i'}{\partial x_j} \right)^2} \quad (16.17)$$

The anelastic form of the thermodynamic energy equation is

$$\rho_0 \left(\frac{\partial \theta}{\partial t} + u_j \frac{\partial \theta}{\partial x_j} \right) = \frac{\theta_0 Q}{T_0 c_p} - \frac{\partial H_j}{\partial x_j} \quad (16.18)$$

where Q represents the sum of all heating processes, and

$$H_j = - \frac{\theta}{T} \kappa \frac{\partial T}{\partial x_j} \quad (16.19)$$

is the flux of θ due to molecular processes. The flux form of (16.18),

$$\frac{\partial(\rho_0 \theta)}{\partial t} + \frac{\partial}{\partial x_j} (u_j \rho_0 \theta + H_j) = \frac{\theta_0}{c_p T_0} Q . \quad (16.20)$$

becomes, after averaging,

$$\frac{\partial}{\partial t}(\rho_0 \bar{\theta}) + \frac{\partial}{\partial x_j}(\rho_0 \bar{u}_j \bar{\theta} + \rho_0 \overline{u'_j \theta'} + \bar{H}_j) = \frac{\theta_0 \bar{Q}}{T_0 c_p}, \quad (16.21)$$

or

$$\rho_0 \left(\frac{\partial \bar{\theta}}{\partial t} + \bar{u}_j \frac{\partial \bar{\theta}}{\partial x_j} \right) = - \frac{\partial}{\partial x_j}(\rho_0 \overline{u'_j \theta'}) + \frac{\theta_0 \bar{Q}}{T_0 c_p} - \frac{\partial \bar{H}_j}{\partial x_j}. \quad (16.22)$$

Subtraction of (16.22) from (16.18) gives

$$\rho_0 \left(\frac{\partial \theta'}{\partial t} + \bar{u}_j \frac{\partial \theta'}{\partial x_j} + u'_j \frac{\partial \bar{\theta}}{\partial x_j} + u'_j \frac{\partial \theta'}{\partial x_j} \right) = \frac{\partial}{\partial x_j}(\rho_0 \overline{u'_j \theta'}) + \frac{\theta_0 Q'}{T_0 c_p} - \frac{\partial H'_j}{\partial x_j}, \quad (16.23)$$

and multiplication by u'_i then yields

$$\begin{aligned} & \rho_0 \left(u'_i \frac{\partial \theta'}{\partial t} + u'_i \bar{u}_j \frac{\partial \theta'}{\partial x_j} + u'_i u'_j \frac{\partial \bar{\theta}}{\partial x_j} + u'_i u'_j \frac{\partial \theta'}{\partial x_j} \right) \\ &= u'_i \frac{\partial}{\partial x_j}(\rho_0 \overline{u'_j \theta'}) + \frac{\theta_0 u'_i Q'}{T_0 c_p} - u'_i \frac{\partial H'_j}{\partial x_j}. \end{aligned} \quad (16.24)$$

Multiplying (16.12) by $\rho_0 \theta'$, adding the result to (16.24), averaging, and combining terms, we obtain a prognostic equation for the potential temperature flux $\rho_0 \overline{u'_i \theta'}$:

$$\begin{aligned} & \frac{\partial}{\partial t}(\rho_0 \overline{u'_i \theta'}) + \frac{\partial}{\partial x_j}(\bar{u}_j \rho_0 \overline{u'_i \theta'} + \overline{u'_j \rho_0 u'_i \theta'}) \\ &= - \rho_0 \overline{u'_i u'_j} \frac{\partial \bar{\theta}}{\partial x_j} - \rho_0 \overline{u'_j \theta'} \frac{\partial \bar{u}_i}{\partial x_j} + 2 \varepsilon_{i,j,k} \rho_0 \overline{u'_j \theta'} \Omega_k \\ & \quad - \rho_0 \theta' \frac{\partial}{\partial x_i} \left(\frac{\delta p'}{\rho_0} \right) + \rho_0 \frac{(\theta')^2}{\theta_0} g_i + \theta' \frac{\partial \mathfrak{T}'_{i,j}}{\partial x_j} + \frac{\theta_0 \overline{u'_i Q'}}{T_0 c_p} - \overline{u'_i \frac{\partial H'_j}{\partial x_j}}. \end{aligned} \quad (16.25)$$

Again, a “triple correlation” has appeared. The heat flux components predicted by (16.25) can be used in (16.14), (16.15), (16.16), and (16.22).

Notice that (16.25) contains $\overline{(\theta')^2}$, which can also be predicted, using

$$\begin{aligned}
& \frac{\partial}{\partial t} \left[\frac{1}{2} \overline{\rho_0 (\theta')^2} \right] + \frac{\partial}{\partial x_j} \left[\overline{u_j \frac{1}{2} \rho_0 (\theta')^2} + \overline{u'_j \frac{1}{2} \rho_0 (\theta')^2} + \overline{H'_j \theta'} \right] \\
& = -\rho_0 \overline{u'_j \theta'} \frac{\partial \bar{\theta}}{\partial x_j} + \frac{\theta_0 \overline{\theta' Q'}}{T_0 c_p} + \overline{H'_j \frac{\partial \theta'}{\partial x_j}}.
\end{aligned} \tag{16.26}$$

Again we see a triple correlation.

In order to complete the second moment equations, we must consider any scalar constituents of the air which are of sufficient interest to warrant prediction. The most important example, and the only one which we shall actually consider, is water in its three phases. A parallel discussion can be given for other chemical constituents, e.g., pollutants.

The average conservation equation for *total* water substance w is

$$\frac{\partial}{\partial t} (\rho_0 \bar{w}) + \frac{\partial}{\partial x_j} (\rho_0 \bar{u_j w} + \rho_0 \overline{u'_j w'} + \bar{W}_j) = \bar{S}_w, \tag{16.27}$$

where \bar{S}_w represents any possible source (or sink) of w (e.g., convergence of precipitation flux), and

$$W_j = -\kappa \frac{\partial w}{\partial x_j} \tag{16.28}$$

is the flux of w due to molecular diffusion. Here we have assumed for simplicity that the molecular diffusion coefficient for water vapor is the same as that for temperature.

By analogy with (16.25), we find that

$$\begin{aligned}
& \frac{\partial}{\partial t} (\rho_0 \overline{u'_i w'}) + \frac{\partial}{\partial x_j} (\overline{u_j \rho_0 u'_i w'} + \overline{u'_j \rho_0 u'_i w'}) = -\rho_0 \overline{u'_i u'_j} \frac{\partial \bar{w}}{\partial x_j} \\
& -\rho_0 \overline{u'_j w'} \frac{\partial \bar{u}}{\partial x_j} + 2\varepsilon_{i,j,k} \rho_0 \overline{u'_j w'} \Omega_k - \rho_0 \overline{w'} \frac{\partial}{\partial x_i} \left(\frac{\delta p'}{\rho_0} \right) + \rho_0 \frac{\overline{w' \theta'}}{\theta_0} g_i \\
& + \overline{w' \frac{\partial \mathfrak{S}'_{i,j}}{\partial x_j}} + \overline{u'_i S'_w} - \overline{u'_i \frac{\partial W'_j}{\partial x_j}}.
\end{aligned} \tag{16.29}$$

The buoyancy term of (16.29) is proportional to the covariance of w and θ , which can be predicted according to

$$\begin{aligned}
\frac{\partial}{\partial t}(\rho_0 \overline{w'\theta'}) + \frac{\partial}{\partial x_j}(\overline{u_j \rho_0 w'\theta'} + \overline{u'_j \rho_0 w'\theta'}) &= -\rho_0 \overline{u'_j \theta'} \frac{\partial \overline{w}}{\partial x_j} \\
&- \rho_0 \overline{u'_j w'} \frac{\partial \overline{\theta}}{\partial x_j} + \frac{\theta_0}{c_p T_0} \overline{w' Q'} + \overline{\theta' S'_w} - \overline{w' \frac{\partial H'_j}{\partial x_j}} - \overline{\theta' \frac{\partial W'_j}{\partial x_j}}.
\end{aligned}
\tag{16.30}$$

We can also derive a prediction equation for $\overline{(w')^2}$. Although this quantity does not appear in any of our other equations, it may be useful to know for other purposes. We include the equation for completeness:

$$\begin{aligned}
\frac{\partial}{\partial t} \left[\frac{1}{2} \overline{\rho_0 (w')^2} \right] + \frac{\partial}{\partial x_j} \left[\overline{u_j \frac{1}{2} \rho_0 (w')^2} + \overline{u'_j \frac{1}{2} \rho_0 (w')^2} + \overline{w' W'_j} \right] \\
= -\rho_0 \overline{u'_j w'} \frac{\partial \overline{w}}{\partial x_j} + \overline{w' S'_w} + \overline{W'_j \frac{\partial w'}{\partial x_j}}.
\end{aligned}
\tag{16.31}$$

16.2.2) Summary

For convenience, we summarize our results in Table 16.1 and Table 16.2.

Mean momentum	$ \begin{aligned} \frac{\partial \overline{u_i}}{\partial t} + \frac{1}{\rho_0} \frac{\partial}{\partial x_j} (\rho_0 \overline{u_i u_j} + \rho_0 \overline{u'_i u'_j} - \overline{\mathfrak{T}_{i,j}}) - 2\varepsilon_{i,j,k} \overline{u_j} \Omega_k \\ = -\frac{\partial}{\partial x_i} \left(\frac{\overline{\delta p}}{\rho_0} \right) + \frac{\overline{\delta \theta}}{\theta_0} g_i \end{aligned} $
Mean continuity	$ \frac{\partial}{\partial x_i} (\rho_0 \overline{u_i}) = 0 $
Mean potential temperature	$ \frac{\partial}{\partial t} (\rho_0 \overline{\theta}) + \frac{\partial}{\partial x_j} (\rho_0 \overline{u_j \theta} + \rho_0 \overline{u'_j \theta'} + \overline{H_j}) = \frac{\theta_0}{c_p T_0} \overline{Q} $
Mean moisture	$ \frac{\partial}{\partial t} (\rho_0 \overline{w}) + \frac{\partial}{\partial x_j} (\rho_0 \overline{u_j w} + \rho_0 \overline{u'_j w'} + \overline{W_j}) = \overline{S_w} $

Table 16.1: The equations for the mean flow.

16.2.3) Discussion

The second moment equations are satisfied if all primed quantities vanish. Therefore, *the equations do not explain why the flow is turbulent*; they only state that any disturbances which arise must satisfy the various interrelationships represented by the

Reynolds stress	$\begin{aligned} \frac{\partial}{\partial t} \left(\rho_0 \overline{u'_i u'_i} \right) + \frac{\partial}{\partial x_j} \left(\rho_0 \overline{u'_j u'_i} \frac{\bar{u}}{2} + \rho_0 \overline{u'_j \frac{1}{2} u'_i u'_i} - \overline{\mathfrak{S}'_{i,j} u'_i} \right) + \frac{\partial}{\partial x_i} (\overline{\delta p' u'_i}) \\ = 2\varepsilon_{i,j,k} \Omega_k \rho_0 \overline{u'_i u'_j} + \frac{\delta p'}{\rho_0} \frac{\partial}{\partial x_i} (\rho_0 \overline{u'_i}) \\ + \frac{\rho_0}{\theta_0} (\overline{u'_i \delta \theta' g_i}) - \rho_0 \overline{u'_i u'_j} \frac{\partial \bar{u}_i}{\partial x_j} - \overline{\mathfrak{S}'_{i,j} \frac{\partial u'_i}{\partial x_j}} \end{aligned}$
TKE equation	$\begin{aligned} \frac{\partial}{\partial t} \left(\rho_0 \overline{\frac{u'^2}{2}} \right) + \frac{\partial}{\partial x_j} \left(\rho_0 \overline{u'_j \frac{u'^2}{2}} + \rho_0 \overline{u'_j \frac{u'^2}{2}} + \overline{\delta p' u'_j} - \overline{u'_i \mathfrak{S}'_{i,j}} \right) = \\ - \rho_0 \overline{u'_i u'_j} \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\rho_0}{\theta_0} \overline{u'_i \delta \theta' g_i} - \overline{\mathfrak{S}'_{i,j} \frac{\partial u'_i}{\partial x_j}} \end{aligned}$
Potential temperature flux	$\begin{aligned} \frac{\partial}{\partial t} (\rho_0 \overline{u'_i \theta'}) + \frac{\partial}{\partial x_j} (\overline{u'_j \rho_0 u'_i \theta'} + \overline{u'_j \rho_0 u'_i \theta'}) \\ = - \rho_0 \overline{u'_i u'_j} \frac{\partial \bar{\theta}}{\partial x_j} - \rho_0 \overline{u'_j \theta'} \frac{\partial \bar{u}_i}{\partial x_j} + 2\varepsilon_{i,j,k} \rho_0 \overline{u'_j \theta'} \Omega_k \\ - \rho_0 \overline{\theta' \frac{\partial (\delta p')}{\partial x_i}} + \rho_0 \overline{\frac{(\theta')^2}{\theta_0} g_i} + \overline{\theta' \frac{\partial \mathfrak{S}'_{i,j}}{\partial x_j}} + \frac{\theta_0 \overline{u'_i Q'}}{T_0 c_p} - \overline{u'_i \frac{\partial H_j}{\partial x_j}} \end{aligned}$
Potential temperature variance	$\begin{aligned} \frac{\partial}{\partial t} \left[\frac{1}{2} \rho_0 \overline{(\theta')^2} \right] + \frac{\partial}{\partial x_j} \left[\overline{u'_j \frac{1}{2} \rho_0 (\theta')^2} + \overline{u'_j \frac{1}{2} \rho_0 (\theta')^2} + \overline{H'_j \theta'} \right] \\ = - \rho_0 \overline{u'_j \theta'} \frac{\partial \bar{\theta}}{\partial x_j} + \frac{\theta_0}{c_p T_0} \overline{\theta' Q'} + \overline{H'_j \frac{\partial \theta'}{\partial x_j}} \end{aligned}$
Moisture flux	$\begin{aligned} \frac{\partial}{\partial t} (\rho_0 \overline{u'_i w'}) + \frac{\partial}{\partial x_j} (\overline{u'_j \rho_0 u'_i w'} + \overline{u'_j \rho_0 u'_i w'}) = - \rho_0 \overline{u'_i u'_j} \frac{\partial \bar{w}}{\partial x_j} \\ - \rho_0 \overline{u'_j w'} \frac{\partial \bar{u}}{\partial x_j} + 2\varepsilon_{i,j,k} \rho_0 \overline{u'_j w'} \Omega_k - \rho_0 \overline{w' \frac{\partial (\delta p')}{\partial x_i}} + \rho_0 \overline{\frac{w' \theta'}{\theta_0} g_i} \\ + \overline{w' \frac{\partial \mathfrak{S}'_{i,j}}{\partial x_j}} + \overline{u'_i S'_w} - \overline{u'_i \frac{\partial W'_j}{\partial x_j}} \end{aligned}$

Table 16.2: The equations for the second moments. The trace of the Reynolds stress equation, i.e. the turbulence kinetic energy equation, is listed separately, for convenience.

Covariance of mixing ratio and potential temperature	$\frac{\partial}{\partial t}(\rho_0 \overline{w'\theta'}) + \frac{\partial}{\partial x_j}(\overline{u_j \rho_0 w'\theta'} + \overline{u'_j \rho_0 w'\theta'})$ $= -\rho_0 \overline{u'_j \theta'} \frac{\partial \overline{w}}{\partial x_j} - \rho_0 \overline{u'_j w'} \frac{\partial \overline{\theta}}{\partial x_j} + \frac{\theta_0}{c_p T_0} \overline{w' Q'} + \overline{\theta' S'_w} - \overline{w' \frac{\partial H'_j}{\partial x_j}} - \overline{\theta' \frac{\partial W'_j}{\partial x_j}}$
Mixing ratio variance	$\frac{\partial}{\partial t} \left[\frac{1}{2} \overline{\rho_0 (w')^2} \right] + \frac{\partial}{\partial x_j} \left[\overline{u_j \frac{1}{2} \rho_0 (w')^2} + \overline{u'_j \frac{1}{2} \rho_0 (w')^2} + \overline{w' W'_j} \right]$ $= -\rho_0 \overline{u'_j w'} \frac{\partial \overline{w}}{\partial x_j} + \overline{w' S'_w} + \overline{W'_j \frac{\partial w'}{\partial x_j}}$

Table 16.2: The equations for the second moments. The trace of the Reynolds stress equation, i.e. the turbulence kinetic energy equation, is listed separately, for convenience.

equations.

It is also important to realize that the “fluctuations” described by the equations need not necessarily be turbulent in any sense. For example, they may be orderly wave motions. Note also that the equations can be used to describe not only laboratory and PBL turbulence, but also ensembles of cumulus clouds, mesoscale convection, and even the effects of zonally asymmetric motions on the zonally-averaged flow.

Finally, as has already been mentioned, the equations are not closed; additional information must be provided if the equations are to be used in models. The unknown terms are of three types: triple moments, second moments involving pressure fluctuations, and second moments involving molecular fluxes.

16.3 Second-order closure

Since the middle 1960s, there has been on-and-off interest, among meteorologists and oceanographers, in modeling the PBL and/or the ocean mixed layer by integrating not only the prediction equations for the mean winds, temperature, moisture, and pollutant concentrations, but also the prediction equations for the turbulent fluxes of these quantities. The predicted fluxes can then be used in the flux convergence terms for the prediction of the mean flow, thus “solving” the problems of parameterizing these fluxes. It has even been suggested that such an approach can be followed in the parameterization of cumulus convection.

As noted above, the problem with this approach is that the second-moment equations involve unknown quantities. Chief among these are all “triple moment” terms, but all terms involving pressure perturbations and all terms involving molecular diffusion are also unknown. These terms have to be “modeled” or “parameterized,” in terms of known quantities.

Donaldson (1973) gives a very readable introduction to this modelling of the prediction equations for the second moments, although the details of his model should be judged against those of his competition. He lists four principles which, he believes, should be applied in devising models of terms of the second-moment equations

- 1) The model must be invariant under an arbitrary transformation of coordinate systems. The model must therefore have all the tensor properties and, in addition, all the symmetries of the term which it replaces.
- 2) The model must be invariant under a Galilean transformation, i.e. if we shift to a second coordinate system which is in constant motion relative to the first, the equations are unchanged.
- 3) The model must have the dimensional properties of the term it replaces.
- 4) The model must be such as to satisfy all the conservation relationships known to govern the variables in question.

All authors mentioned here use the “tendency-towards-isotropy” model of the pressure-shear covariance terms of the Reynolds stress equation, i.e.

$$\frac{\partial}{\partial t}(\rho_0 \overline{u'_i u'_l}) \sim \left(\frac{\delta p'}{\rho_0} \left[\frac{\partial}{\partial x_i}(\rho_0 u'_l) + \frac{\partial}{\partial x_l}(\rho_0 u'_i) \right] = \frac{-q}{3l_1} \left(\overline{u'_i u'_l} - \frac{\delta_{il}}{3} q^2 \right) \right), \quad (16.32)$$

where

$$q^2 = \overline{u'_k u'_k} \equiv 2e, \quad (16.33)$$

and l_1 is a length scale which has to be prescribed. If the turbulence is truly isotropic, then only the diagonal members of $\overline{u'_i u'_l}$ are non-zero (because the others are *fluxes*), and these three diagonal members must each be equal to $\frac{1}{3}q^2$, so that $\overline{u'_i u'_l} - \frac{\delta_{il}}{3}q^2$, which appears on the right-hand-side of (16.32), will vanish. The term is thus formulated as a measure of the departure from isotropy. Notice that if $\overline{u'_i u'_l}$ departs from its isotropic value (0 for the off-diagonal members, and $\frac{1}{3}q^2$ for the diagonal members), then the term will tend to force it back towards isotropy. One effect of this is that the Reynolds stresses can't become too large. This model of the term stems from the recognition that the pressure-shear covariance terms only redistribute kinetic energy among the three components. It was first suggested by Rotta (1951).

In a similar way, we take

$$\overline{p' \frac{\partial \theta'}{\partial x_i}} = -\frac{q}{3l_2} (\overline{u'_i \theta'}) , \quad (16.34)$$

and

$$\overline{p' \frac{\partial w'}{\partial x_i}} = -\frac{q}{3l_3} (\overline{u'_i w'}) , \quad (16.35)$$

in the prediction equations for $\overline{\rho_0 u'_i \theta'}$ and $\overline{\rho_0 u'_i w'}$ respectively.

The remaining terms of these equations which involve p' are all derivatives, and so should tend to vanish when integrated over sufficiently large regions. They are therefore modelled as transport terms.

$$\overline{p' u'_k} \sim -\rho_0 \lambda_1 q \frac{\partial}{\partial x_i} (\overline{u'_i u'_k}) , \quad (16.36)$$

$$\overline{p' \theta'} \sim -\rho_0 \lambda_1 q \frac{\partial}{\partial x_i} (\overline{u'_i \theta'}) , \quad (16.37)$$

$$\overline{p' w'} \sim -\rho_0 \lambda_1 q \frac{\partial}{\partial x_i} (\overline{u'_i w'}) . \quad (16.38)$$

The “triple correlation” terms of the forecast equations are also transport terms. The total model is then

$$\begin{aligned} & -\frac{\partial}{\partial x_j} (\rho_0 \overline{u'_i u'_j u'_l}) - \frac{\partial}{\partial x_i} (\overline{u'_l p'}) - \frac{\partial}{\partial x_l} (\overline{u'_i p'}) = \\ & \frac{\partial}{\partial x_k} \left\{ q \lambda_1 \left[\frac{\partial}{\partial x_k} (\rho_0 \overline{u'_i u'_l}) + \frac{\partial}{\partial x_i} (\rho_0 \overline{u'_l u'_k}) + \frac{\partial}{\partial x_l} (\rho_0 \overline{u'_k u'_i}) \right] \right\} , \end{aligned} \quad (16.39)$$

$$-\frac{\partial}{\partial x_j} (\overline{u'_j \rho_0 u'_i w'}) - \rho_0 \frac{\partial}{\partial x_i} \left(\frac{\overline{p' w'}}{\rho_0} \right) = \frac{\partial}{\partial x_k} \left\{ q \lambda_4 \left[\frac{\partial}{\partial x_k} (\rho_0 \overline{u'_i w'}) + \frac{\partial}{\partial x_i} (\rho_0 \overline{u'_i w'}) \right] \right\} . \quad (16.40)$$

Similarly, the triple correlation terms of the scalar variance and covariance forecast equations are modelled as down-gradient diffusion terms:

$$-\frac{\partial}{\partial x_j} \left[\overline{u'_j \frac{1}{2} \rho_0 (\theta')^2} \right] = \frac{\partial}{\partial x_k} \left\{ q \lambda_2 \frac{\partial}{\partial x_k} \left[\frac{1}{2} \rho_0 (\theta')^2 \right] \right\}, \quad (16.41)$$

$$-\frac{\partial}{\partial x_j} (\overline{u'_j \rho_0 w' \theta'}) = \frac{\partial}{\partial x_k} \left[q \lambda_5 \frac{\partial}{\partial x_k} (\rho_0 w' \theta') \right], \quad (16.42)$$

$$-\frac{\partial}{\partial x_j} \left[\overline{u'_j \frac{1}{2} \rho_0 (w')^2} \right] = \frac{\partial}{\partial x_k} \left\{ q \lambda_6 \frac{\partial}{\partial x_k} \left[\frac{1}{2} \rho_0 (w')^2 \right] \right\}. \quad (16.43)$$

All of these modelling assumptions are “safe;” the modelled terms will not blow up in a computer simulation. None of the modelling assumptions are very convincing -- no more convincing than the mixing length theory that they replace. There is what Lumley calls an “article of faith,” that weak assumptions at third order are preferable to weak assumptions at second order. As discussed later, the results are rather convincing.

The dissipation terms of the variance production equations are modelled as exponential decay, while all other molecular terms are neglected:

$$-\frac{\overline{\mathfrak{S}'_{i,j} \partial u'_l}}{\rho_0 \partial x_j} - \frac{\overline{\mathfrak{S}'_{l,j} \partial u'_i}}{\rho_0 \partial x_j} = -\frac{2q^3}{3\Lambda_1} \delta_{il}, \quad (16.44)$$

$$\frac{\partial}{\partial x_j} (\overline{u'_l \mathfrak{S}'_{i,j}} + \overline{u'_i \mathfrak{S}'_{l,j}}) = 0, \quad (16.45)$$

$$\overline{\theta' \frac{\partial \mathfrak{S}'_{i,j}}{\partial x_j}} - \overline{u'_i \frac{\partial H'_j}{\partial x_j}} = 0, \quad (16.46)$$

$$\overline{H'_j \frac{\partial \theta'}{\partial x_j}} = -\frac{2q}{\Lambda_2} \overline{(\theta')^2}, \quad (16.47)$$

$$-\frac{\partial}{\partial x_j} (\overline{H'_j \theta'}) = 0, \quad (16.48)$$

$$-\overline{u'_i \frac{\partial W'_j}{\partial x_j}} = 0, \quad (16.49)$$

$$-\overline{w' \frac{\partial H'_j}{\partial x_j}} - \overline{\theta' \frac{\partial W'_j}{\partial x_j}} = 0 , \quad (16.50)$$

$$\overline{W'_j \frac{\partial w'}{\partial x_j}} = -\frac{2q}{\Lambda_3} \overline{(w')^2} , \quad (16.51)$$

$$-\frac{\partial}{\partial x_j} (\overline{W'_j w'}) = 0 . \quad (16.52)$$

The heating and moistening terms are usually ignored:

$$\frac{\theta_0}{T_0} \overline{u'_i Q'} = 0 , \quad (16.53)$$

$$\frac{\theta_0}{T_0} \overline{\theta' Q'} = 0 , \quad (16.54)$$

$$\overline{u'_i S'_w} = 0 , \quad (16.55)$$

$$\frac{\theta_0}{T_0} \overline{w' Q'} + \overline{\theta' S'_w} = 0 , \quad (16.56)$$

$$\overline{w' S'_w} = 0 . \quad (16.57)$$

No one argues that they are negligible in all cases, although no doubt they are in some. Their potential importance must be faced where the equations are applied to clouds.

In most theories, all of the various length scales introduced above are assumed to be proportional to each other, and the proportionality factors are assumed to be constants. The models are “tuned” by choice of these constants. Usually no attempt is made to argue that the constants are “universal,” although it is openly (but tacitly) assumed that they are.

A variety of different closure theories can be constructed by choice of retained terms in the equations. We now survey a few of these theories.

Mellor and Yamada (1974) presented a hierarchy of turbulence closure models, ranging from a fully prognostic system of second-moment equations (Level 4) to a fully diagnostic subset corresponding to mixing length theory (Level 1). These are summarized in Table 16.3. None of the models includes molecular effects other than dissipation, or diabatic effects, or coriolis effects (except in the equation of mean motion), or buoyant

Level 4	Reynolds stress tensor (six equations) $\overline{(\theta')^2}$ (one equation) Heat flux vector (three equations)
Level 3	Turbulence kinetic energy (one equation) $\overline{(\theta')^2}$ (one equation)
Level 2	None
Level 1	None

Table 16.3: Prognostic variables of the dry Mellor–Yamada models.

production of momentum, heat, and moisture fluxes. All of the models are Boussinesq (up to now we have used the anelastic system). Level 4 then includes 15 differential equations for the second moments, in addition to 5 for the mean flow. Of course, modeling of pollutant transport would require additional equations. At Level 3, only three differential equations are used for the second moments - those for e , $\overline{(\theta')^2}$, and $\overline{(w')^2}$. Levels 2 and 1 involve only diagnostic relations for all of the second moments. Level 1 turns out to be equivalent to the “mixing length” theory.

Mellor and Yamada experimented with each of the models, and concluded that in most applications the additional realism obtained at Level 4 was not sufficiently better than that at Level 3 to warrant the additional computational complexity. Of course, this conclusion is based in part on the parameterizations that they used for the triple moments, the dissipation terms, and the pressure terms.

Wyngaard and Coté (1974) and Wyngaard (1975) applied a simplified version of the Lumley-Khajeh-Nouri model to the simulation of both the unstable and the stable PBLs, comparing their results to the Wangara and Minnesota observations, and to the more detailed calculations of Deardorff.

16.4 The third-moment equations

An equation to predict $\overline{w'w'w'}$ can be derived by using

$$\frac{\partial}{\partial t} \overline{w'w'w'} = 3 \overline{w'w'} \frac{\partial}{\partial t} \overline{w'}. \quad (16.58)$$

Here $w' \equiv u'_3$; in the following, we also use $z \equiv x_3$, and we replace g_i by g . From (16.12) we find that

$$\begin{aligned} \frac{\partial w'}{\partial t} + \bar{u}_j \frac{\partial}{\partial x_j} w' + u'_j \frac{\partial \bar{w}}{\partial x_j} + u'_j \frac{\partial}{\partial x_j} w' = \\ 2\varepsilon_{3,j,k} u'_j \Omega_k - \frac{\partial}{\partial z} \left(\frac{\delta p'}{\rho_0} \right) + \frac{\delta \theta'}{\theta_0} g + \frac{1}{\rho_0} \frac{\partial}{\partial x_j} (\mathfrak{T}'_{3,j} - \rho_0 \overline{w' u'_j}). \end{aligned} \quad (16.59)$$

After multiplication by $3w'w'$, we obtain:

$$\begin{aligned} \frac{\partial}{\partial t} w'w'w' + \bar{u}_j \frac{\partial}{\partial x_j} w'w'w' + 3w'w'u'_j \frac{\partial \bar{w}}{\partial x_j} + u'_j \frac{\partial}{\partial x_j} w'w'w' = \\ 6\varepsilon_{3,j,k} u'_j w'w' \Omega_k - 3w'w' \frac{\partial}{\partial z} \left(\frac{\delta p'}{\rho_0} \right) + 3 \frac{g}{\theta_0} w'w' \delta \theta' + \frac{3w'w'}{\rho_0} \frac{\partial}{\partial x_j} (\mathfrak{T}'_{3,j} - \rho_0 \overline{w' u'_j}). \end{aligned} \quad (16.60)$$

Use of the continuity equation for the fluctuating part of the flow, and averaging, introduces a “fourth moment” term:

$$\begin{aligned} \frac{\partial}{\partial t} \overline{w'w'w'} + \bar{u}_j \frac{\partial}{\partial x_j} \overline{w'w'w'} + 3 \overline{w'w'u'_j} \frac{\partial \bar{w}}{\partial x_j} + \frac{1}{\rho_0} \frac{\partial}{\partial x_j} (\rho_0 \overline{u'_j w'w'w'}) = \\ 6\varepsilon_{i,j,k} \overline{u'_j w'w'} \Omega_k - 3 \overline{w'w'} \frac{\partial}{\partial z} \left(\frac{\delta p'}{\rho_0} \right) + 3 \frac{g_i}{\theta_0} \overline{w'w'} \delta \theta' \\ + \frac{3}{\rho_0} \overline{w'w'} \frac{\partial \mathfrak{T}'_{3,j}}{\partial x_j} - \frac{3 \overline{w'w'}}{\rho_0} \frac{\partial}{\partial x_j} (\rho_0 \overline{w' u'_j}) . \end{aligned} \quad (16.61)$$

Normally this is simplified by neglecting advection by the mean flow, the production term involving $\frac{\partial w}{\partial x_j}$, the rotation term, and $\frac{3 \overline{w'w'}}{\rho_0} \frac{\partial}{\partial x_j} (\rho_0 \overline{w' u'_j})$:

$$\begin{aligned} \frac{\partial}{\partial t} \overline{w'w'w'} + \frac{1}{\rho_0} \frac{\partial}{\partial x_j} (\rho_0 \overline{u'_j w'w'w'}) = \\ - 3 \overline{w'w'} \frac{\partial}{\partial z} \left(\frac{\delta p'}{\rho_0} \right) + 3 \frac{g_i}{\theta_0} \overline{w'w'} \delta \theta' + \frac{3}{\rho_0} \overline{w'w'} \frac{\partial \mathfrak{T}'_{3,j}}{\partial x_j} . \end{aligned} \quad (16.62)$$

16.5 Third- order closure

André and collaborators (1976 a, b, 1978) constructed a model in which the third moments are predicted, and the fourth moments are expanded in terms of the second moments through the quasi-normal approximation:

$$\overline{a'b'c'd'} \cong \overline{a'b'} \overline{c'd'} + \overline{a'c'} \overline{b'd'} + \overline{a'd'} \overline{b'c'} , \quad (16.63)$$

which is exact if a , b , c and d are Gaussian random variables. It has been shown that models based on this idea predict the development of negative variances, and other non-physical behavior. André et al. suggested that the difficulty can be avoided by requiring that the third moments satisfy Schwartz's inequality, which can be expressed as

$$|\overline{a'b'c'}| \leq \min \left\{ \begin{aligned} &\left\{ \overline{a^2 [b^2 \overline{c'^2} + (\overline{b'c'})^2]} \right\}^{1/2} \\ &\left\{ \overline{b^2 [a^2 \overline{c'^2} + (\overline{a'c'})^2]} \right\}^{1/2} \\ &\left\{ \overline{c^2 [a^2 \overline{b'^2} + (\overline{a'b'})^2]} \right\}^{1/2} \end{aligned} \right\}. \quad (16.64)$$

This is called a “realizability” constraint.

Third-moment closure is being used in some high-resolution cloud models (e.g. Krueger 1988).

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