Where Do Fluxes Come From?

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1 Four closures needed

A key 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.

This essay derives and discusses a set of equations that governs these various statistics. The method is often called "higher-order closure," for reasons that will become clear. The basic equations of higher-order closure can be applied to any type of motion, including turbulence, cumulus convection, and gravity waves. This extreme generality is an attraction of the method. Unfortunately, the closures needed for actual use of the equations are not comparably general.

In statistical parlance, the average of a field (e.g., the potential temperature) is called a "first moment." The second moment is the average of the square of the field, but we will use the term second moment to refer to "second moments about the mean," which are the averages of products of two departures from the mean(s) of one or more variables; these are variances and covariances. Third moments are averages of the products of three departures from the mean, and so on. The examples given later will make the terminology more clear. As will be explained, the equations that predict the first moments involve the second moments, equations to predict the second moments involve the third moments, and so on. This is one of the four closure problems of turbulence.

The second closure problem is that the equations used to predict statistics involving velocity components inevitably include statistics that involve the pressure field; these represent additional unknowns.

The third closure problem is that the equations for the second (and higher) moments include important terms arising from molecular viscosity and molecular conductivity. These involve unknown statistics of the very small-scale spatial structure.

The fourth closure problem is parameterizing the source and sink terms, due to such processes as phase changes and radiative heating.

In the following sections, we will discuss the first the first and second moments of the winds, the potential temperature, and moisture. We will also briefly discuss some third and fourth moments.

2 The starting point

The anelastic momentum equation can be written in flux form as

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

Here $\delta p = p - p_0$, $\delta\theta \equiv \theta - \theta_0$, and $\mathscr{F}$ is the viscous stress tensor. By convention, repeated subscripts are summed out. 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. Here "otherwise" refers to the case in which two or more of the subscripts take the same numerical value. In somewhat simplified form, the viscous stress tensor can be expanded as

$$\mathscr{F}_{i,j} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\mu\delta_{i,j}\frac{\partial u_k}{\partial x_k}, \tag{2}$$

where μ is the molecular viscosity and $\delta_{i,j}$ is the Kroneker delta. Note that $\frac{\partial u_k}{\partial x_k}$ is simply the divergence of the wind vector, and appears in the same way in each element of $\mathscr{F}$. The sum of the diagonal elements of $\mathscr{F}$ satisfies

$$\mathscr{F}_{i,i} = 2\mu\left(\frac{\partial u_i}{\partial x_i} - \frac{1}{3}\frac{\partial u_k}{\partial x_k}\right) = 0. \tag{3}$$

The anelastic continuity equation is

$$\frac{\partial}{\partial x_i}\left(\rho_0 u_i\right) = 0. \tag{4}$$

Using (4), we can rewrite the momentum equation in advective form:

$$\frac{\partial u_i}{\partial t} + u_j\frac{\partial u_i}{\partial x_j} - \frac{1}{\rho_0}\frac{\partial \mathscr{F}_{i,j}}{\partial x_j} - 2\varepsilon_{i,j,k}u_j\Omega_k = -\frac{\partial}{\partial x_i}\left(\frac{\delta p}{\rho_0}\right) + \frac{\delta\theta}{\theta_0}g_i. \tag{5}$$

The anelastic form of the thermodynamic energy equation is

$$\rho_0\left(\frac{\partial\theta}{\partial t} + u_j\frac{\partial\theta}{\partial x_j}\right) = \frac{\theta_0}{T_0}\frac{Q}{c_p} - \frac{\partial H_j}{\partial x_j} \tag{6}$$

where Q represents the sum of all heating processes, and

$$H_j = -\frac{\theta}{T}\kappa\frac{\partial T}{\partial x_j} \tag{7}$$

is the flux of θ due to molecular processes. The flux form of (6) is

$$\frac{\partial(\rho_0\theta)}{\partial t} + \frac{\partial}{\partial x_j}(u_j\rho_0\theta + H_j) = \frac{\theta_0}{c_p T_0}Q \tag{8}$$

Finally, the conservation equation for total water substance is

$$\rho_0\left(\frac{\partial q_t}{\partial t} + u_j\frac{\partial q_t}{\partial x_j}\right) + \frac{\partial W_j}{\partial x_j} = S_w, \tag{9}$$

where S_w represents any possible source (or sink) of q_t (e.g., convergence of precipitation flux), and

$$W_j = -\kappa\frac{\partial q_t}{\partial x_j} \tag{10}$$

is the flux of q_t due to the molecular diffusion of water vapor. Here we have assumed for simplicity that the molecular diffusion coefficient for water vapor is the same as that for temperature. The flux form corresponding to (9) is

$$\frac{\partial(\rho_0 q_t)}{\partial t} + \frac{\partial}{\partial x_j}(u_j\rho_0 q_t + W_j) = S_w. \tag{11}$$

3 Averaging the continuity equation

The Reynolds decomposition,

$$() = \overline{()} + ()' \tag{12}$$

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

$$\frac{\partial}{\partial x_i}\left(\rho_0 \bar{u}_i\right) = 0. \tag{13}$$

Here $\bar{u}_i$ is an example of a "first moment." We can then use (4) and (12) to write the continuity equation for the fluctuations as

$$\frac{\partial}{\partial x_i}\left(\rho_0 u_i'\right) = 0. \tag{14}$$

We will need both (13) and (14) in the following analysis.

4 Averaging the momentum equation

Averaging (1) gives us the equation of motion for the mean flow:

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{1}{\rho_0}\frac{\partial}{\partial x_j}\left(\rho_0 \bar{u}_i \bar{u}_j + \rho_0 \overline{u_i' u_j'} - \overline{\mathscr{F}_{i,j}}\right) - 2\varepsilon_{i,j,k}\bar{u}_j \Omega_k = -\frac{\partial}{\partial x_i}\left(\frac{\overline{\delta p}}{\rho_0}\right) + \frac{\overline{\delta\theta}}{\theta_0} g_i \tag{15}$$

Here we have used the usual Reynolds averaging result that

$$\overline{u_i u_j} = \bar{u}_i \bar{u}_j + \overline{u_i' u_j'}. \tag{16}$$

In (15), the new quantity $\rho_0 \overline{u_i' u_j'}$ is called the "Reynolds stress;" it appears in parallel with the viscous stress, but it is normally many orders of magnitude larger than the viscous stress. The quantity $\overline{u_i' u_j'}$, which is the main ingredient of the Reynolds stress, is an example of a "second moment." The Reynolds stress can also be called the turbulent momentum flux. It is a tensor, because it is associated with "two directions:" the direction of the momentum vector that is being transported, and the direction in which it is being carried. Using the averaged continuity equation, (13), Eq. (15) can also be written in the "advective form:"

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} + \frac{1}{\rho_0}\frac{\partial}{\partial x_j}\left(\rho_0 \overline{u_i' u_j'} - \overline{\mathscr{F}_{i,j}}\right) - 2\varepsilon_{i,j,k}\bar{u}_j \Omega_k = -\frac{\partial}{\partial x_i}\left(\frac{\overline{\delta p}}{\rho_0}\right) + \frac{\overline{\delta\theta}}{\theta_0} g_i. \tag{17}$$

5 The Reynolds stress equation

We now begin a discussion of the prediction equations for the second moments, starting with the most complicated case, which arises from the momentum equation.

Subtracting (17) from the advective form of the un-averaged momentum equation, (5), using (12) and (14), and rearranging, we obtain the momentum equation for the fluctuating part of the wind field:

$$\begin{aligned} &\frac{\partial u_i'}{\partial t} + \bar{u}_j \frac{\partial u_i'}{\partial x_j} + u_j{}' \frac{\partial \bar{u}_i}{\partial x_j} + \frac{1}{\rho_0} \frac{\partial}{\partial x_j} \left(\rho_0 u_i' u_j' - \rho_0 \overline{u_i' u_j'} \right) - \frac{1}{\rho_0} \frac{\partial \mathscr{F}_{i,j}'}{\partial x_j} - 2\varepsilon_{i,j,k} u_j' \Omega_k \\ &= -\frac{\partial}{\partial x_i} \left(\frac{\delta p'}{\rho_0} \right) + \frac{\delta \theta'}{\theta_0} g_i. \end{aligned} \tag{18}$$

Deriving (18) is a little bit tricky, so you should work it through to see how it goes. Inspection of (18) shows that each term will vanish if averaged. Multiplying (18) by $\rho_0 u_l'$ gives

$$\begin{aligned} &\rho_0 u_l' \frac{\partial u_i'}{\partial t} + \rho_0 u_l' \bar{u}_j \frac{\partial u_i'}{\partial x_j} + \rho_0 u_l' u_j{}' \frac{\partial \bar{u}_i}{\partial x_j} + u_l' \frac{\partial}{\partial x_j} \left(\rho_0 u_i' u_j' - \rho_0 \overline{u_i' u_j'} \right) - u_l' \frac{\partial \mathscr{F}_{i,j}'}{\partial x_j} - 2\rho_0 u_l' \varepsilon_{i,j,k} u_j' \Omega_k \\ &= -\rho_0 u_l' \frac{\partial}{\partial x_i} \left(\frac{\delta p'}{\rho_0} \right) + \rho_0 u_l' \frac{\delta \theta'}{\theta_0} g_i. \end{aligned} \tag{19}$$

Of course, (19) remains valid if i and l are interchanged. Performing this operation, adding the result to (19), averaging, and combining terms, we obtain the Reynolds stress equation:

$$
\begin{aligned}
&\frac{\partial}{\partial t}\left(\rho_0\overline{u_i'u_l'}\right)+\frac{\partial}{\partial x_j}\left(\rho_0\bar{u}_j\overline{u_i'u_l'}+\rho_0\overline{u_i'u_j'u_l'}-\overline{u_i'\mathscr{F}_{l,j}'}-\overline{u_l'\mathscr{F}_{i,j}'}\right)\\
&-2\varepsilon_{l,j,k}\Omega_k\rho_0\overline{u_i'u_j'}-2\varepsilon_{i,j,k}\Omega_k\rho_0\overline{u_l'u_j'}\\
=&-\rho_0\overline{u_l'u_j'}\frac{\partial\bar{u}_i}{\partial x_j}-\rho_0\overline{u_i'u_j'}\frac{\partial\bar{u}_l}{\partial x_j}\\
&-\frac{\partial}{\partial x_i}\left(\overline{u_l'\delta p'}\right)-\frac{\partial}{\partial x_l}\left(\overline{u_i'\delta p'}\right)+\overline{\frac{\delta p'}{\rho_0}\frac{\partial}{\partial x_i}\left(\rho_0u_l'\right)}+\overline{\frac{\delta p'}{\rho_0}\frac{\partial}{\partial x_l}\left(\rho_0u_i'\right)}\\
&+\frac{\rho_0}{\theta_0}\left(\overline{u_l'\delta\theta'}g_i+\overline{u_i'\delta\theta'}g_l\right)-\left(\overline{\mathscr{F}_{i,j}'\frac{\partial u_l'}{dx_j}}+\overline{\mathscr{F}_{l,j}'\frac{\partial u_i'}{\partial x_j}}\right).
\end{aligned}
\tag{20}
$$

In deriving (20), we have used both of the two continuity equations, (13) and (14).

We see from (20) that the present value of $\rho_0\overline{u_i'u_l'}$ depends on its past history. If (20) is used to predict $\rho_0\overline{u_i'u_l'}$, then the result can be used to predict $\bar{u}_i$, using (15) or (17). There are three "closure" problems, however: First of all, Eq. (20) contains the new unknown $\rho_0\overline{u_i'u_j'u_l'}$ (a "triple correlation," or "third moment"), which must be determined before $\rho_0\overline{u_i'u_l'}$ can be predicted. In addition, (20) contains second moments involving the pressure, and second moments involving the viscous stress tensor. There are "two kinds" of pressure terms, and two kinds of viscous terms. The viscous terms appear on both the right- and left-hand sides of (20). We conclude that three closures are needed before (20) can be used: closures for the third moments, closures for the pressure terms, and closures for the viscous terms.

It is possible to derive a prognostic equation for the triple moment $\rho_0\overline{u_i'u_j'u_l'}$, but it contains fourth moments, etc. One strategy is to model or parameterize the third moments in terms of the mean flow and the second moments. Some success has been achieved with this approach, which is called "second-order closure." Further discussion of the third moments is given later.

6 The turbulence kinetic energy equation

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

$$\frac{\partial}{\partial t}\left(\rho_0\frac{\overline{u_i'u_i'}}{2}\right)+\frac{\partial}{\partial x_j}\left(\rho_0\bar{u}_j\frac{\overline{u_i'u_i'}}{2}+\overline{\rho_0 u_j'\frac{1}{2}u_i'u_i'}-\overline{\mathscr{F}_{l,j}'u_i'}\right)+\frac{\partial}{\partial x_i}\left(\overline{\delta p' u_i'}\right)-2\varepsilon_{i,j,k}\Omega_k\rho_0\overline{u_i'u_j'}$$
$$=\overline{\frac{\delta p'}{\rho_0}\frac{\partial}{\partial x_i}\left(\rho_0 u_i'\right)}+\frac{\rho_0}{\theta_0}\left(\overline{u_i'\delta\theta'}g_i\right)-\rho_0\overline{u_i'u_j'}\frac{\partial\bar{u}_i}{\partial x_j}-\overline{\mathscr{F}_{i,j}'\frac{\partial u_i'}{\partial x_j}}\ . \tag{21}$$

Here we temporarily suspend the summation convention for the *i* subscript only, so that (21) represents three equations for the three velocity variances $\rho_0\frac{\overline{u'_1u'_1}}{2}$, $\rho_0\frac{\overline{u'_2u'_2}}{2}$, and $\rho_0\frac{\overline{u'_3u'_3}}{2}$.

We have moved one of the pressure terms to the left-hand side of (21), because it represents energy transport by pressure-work. The other pressure term, on the right-hand side of the equation, will be discussed below.

Similarly, the viscous terms on the left-hand side of (21) represent energy transports by the viscous force; they do not act as net sources or sinks. In contrast, the viscous terms on the right-hand side of (21) represent net sinks of the velocity variances; this can be seen by use of (2). They are called "dissipation" terms.

The rotation and pressure terms on the second line of (21) merely redistribute energy among the three individual components, e.g., from $\frac{1}{2}\overline{u'_1u'_1}$ to $\frac{1}{2}\overline{u'_2u'_2}$. This means that they will cancel out when we sum (21) over *i*. The pressure term is usually larger than the rotation term, and will be discussed further below. The rotation term may be important for mesoscale Reynolds stresses.

Now reinstating the summation convention, we "contract" (21) to obtain the turbulence kinetic energy (TKE) equation:

$$\boxed{\begin{aligned}&\frac{\partial}{\partial t}\left(\rho_0\frac{\overline{u_i'^2}}{2}\right)+\frac{\partial}{\partial x_j}\left(\rho_0\bar{u}_j\frac{\overline{u_i'^2}}{2}+\overline{\rho_0 u_j'\frac{u_i'^2}{2}}+\overline{\delta p' u_j'}-\overline{u_i'\mathscr{F}_{i,j}'}\right)\\&=-\rho_0\overline{u_i'u_j'}\frac{\partial\bar{u}_i}{\partial x_j}+\frac{\rho_0}{\theta_0}\overline{u_i'\delta\theta' g_i}-\overline{\mathscr{F}_{i,j}'\frac{\partial u_i'}{\partial x_j}}.\end{aligned}} \tag{22}$$

Note that the rotation and pressure-redistribution terms have cancelled, because they only redistribute energy.

The terms in $\frac{\partial}{\partial x_j}()$ on the left-hand side of (22) 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 (2) to write

$$\overline{\mathscr{F}'_{i,j}\frac{\partial u'_i}{\partial x_j}} = \mu\overline{\left(\frac{\partial u'_i}{\partial x_j}\right)^2}. \tag{23}$$

The TKE equation is by far the most widely used of the second-moment equations. Many models predict the TKE, and then use it in diagnostic closure assumptions to determine the fluxes that appear in the first-moment equations.

7 The second- and third-moment equations for generic scalars

Consider a generic scalar variable, A, satisfying

$$\rho_0\left(\frac{\partial A}{\partial t} + u_j\frac{\partial A}{\partial x_j}\right) + \frac{\partial}{\partial x_j}(M_A)_j = S_A. \tag{24}$$

where is a source of , per unit volume, and is the (vector) molecular flux of . The corresponding flux form is

$$\frac{\partial(\rho_0 A)}{\partial t} + \frac{\partial}{\partial x_j}\left[u_j\rho_0 A + (M_A)_j\right] = S_A. \tag{25}$$

Reynolds-averaging (25) gives

$$\frac{\partial(\rho_0 A)}{\partial t} + \frac{\partial}{\partial x_j}\left[u_j\rho_0 A + (M_A)_j\right] = S_A. \tag{26}$$

The corresponding advective form is

$$\rho_0\left(\frac{\partial\overline{A}}{\partial t} + \overline{u_j}\frac{\partial\overline{A}}{\partial x_j}\right) + \frac{\partial}{\partial x_j}\left[\rho_0\overline{u'_j A'} + \left(\overline{M_A}\right)_j\right] = \overline{S_A}. \tag{27}$$

Subtracting (27) from (24), we find that

$$\rho_0\left(\frac{\partial A'}{\partial t}+\bar{u}_j\frac{\partial A'}{\partial x_j}+u'_j\frac{\partial\overline{A}}{\partial x_j}+u'_j\frac{\partial A'}{\partial x_j}\right)+\frac{\partial}{\partial x_j}\left[-\rho_0\overline{u'_jA'}+\left(M'_A\right)_j\right]=S'_A. \tag{28}$$

Similarly, a second generic scalar, B, satisfies

$$\rho_0\left(\frac{\partial B'}{\partial t}+\bar{u}_j\frac{\partial B'}{\partial x_j}+u'_j\frac{\partial\overline{B}}{\partial x_j}+u'_j\frac{\partial B'}{\partial x_j}\right)+\frac{\partial}{\partial x_j}\left[-\rho_0\overline{u'_jB'}+\left(M'_B\right)_j\right]=S'_B. \tag{29}$$

Multiplying (28) by B', and (29) by A', and adding the results, we find that

$$\begin{aligned}\rho_0\left[\frac{\partial}{\partial t}\left(A'B'\right)+\bar{u}_j\frac{\partial}{\partial x_j}\left(A'B'\right)+u'_jB'\frac{\partial\overline{A}}{\partial x_j}+u'_jA'\frac{\partial\overline{B}}{\partial x_j}+u'_j\frac{\partial}{\partial x_j}\left(A'B'\right)\right]\\+B'\frac{\partial}{\partial x_j}\left[-\rho_0\overline{u'_jA'}+\left(M'_A\right)_j\right]+A'\frac{\partial}{\partial x_j}\left[-\rho_0\overline{u'_jB'}+\left(M'_B\right)_j\right]=B'S'_A+A'S'_B.\end{aligned} \tag{30}$$

Use of the two continuity equations (13) and (14) allows us to rewrite (30) as

$$\begin{aligned}\frac{\partial}{\partial t}\left(\rho_0A'B'\right)+\frac{\partial}{\partial x_j}\left(\rho_0\bar{u}_jA'B'+\rho_0u'A'B'\right)+\rho_0u'_jB'\frac{\partial\overline{A}}{\partial x_j}+\rho_0u'_jA'\frac{\partial\overline{B}}{\partial x_j}\\+B'\frac{\partial}{\partial x_j}\left[-\rho_0\overline{u'_jA'}+\left(M'_A\right)_j\right]+A'\frac{\partial}{\partial x_j}\left[-\rho_0\overline{u'_jB'}+\left(M'_B\right)_j\right]=B'S'_A+A'S'_{BB}\ .\end{aligned} \tag{31}$$

Reynolds-averaging (31) gives

$$\begin{aligned}\frac{\partial}{\partial t}\left(\rho_0\overline{A'B'}\right)+\frac{\partial}{\partial x_j}\left(\rho_0\bar{u}_j\overline{A'B'}+\rho_0\overline{u'A'B'}\right)+\rho_0\overline{u'_jB'}\frac{\partial\overline{A}}{\partial x_j}+\rho_0\overline{u'_jA'}\frac{\partial\overline{B}}{\partial x_j}\\+\overline{B'\frac{\partial}{\partial x_j}\left[\left(M'_A\right)_j\right]}+\overline{A'\frac{\partial}{\partial x_j}\left[\left(M'_B\right)_j\right]}=\overline{B'S'_A}+\overline{A'S'_B}\ .\end{aligned} \tag{32}$$

Finally, we move the gradient-production terms to the right-hand side, and rearrange the molecular terms to separate the transport from the dissipation. The result is

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\rho_0\overline{A'B'}\right)+\frac{\partial}{\partial x_j}\left[\rho_0\bar{u}_j\overline{A'B'}+\rho_0\overline{u'A'B'}+\overline{B'(M'_A)_j}+\overline{A'(M'_B)_j}\right]\\&=-\rho_0\overline{u'_jB'}\frac{\partial\overline{A}}{\partial x_j}-\rho_0\overline{u'_jA'}\frac{\partial\overline{B}}{\partial x_j}+\overline{B'S'_A}+\overline{A'S'_B}+\overline{(M'_A)_j\frac{\partial B'}{\partial x_j}}+\overline{(M'_B)_j\frac{\partial A'}{\partial x_j}}\end{aligned}\tag{33}$$

The molecular transport terms of (33) are normally negligible. The molecular dissipation terms may or may not be negligible.

In a similar way, we can derive a generic third-moment equation governing $\overline{A'B'C'}$, where C is a third generic scalar. As a starting point, we use the product rule for differentiation to write

$$\begin{aligned}\frac{\partial}{\partial t}\left(A'B'C'\right)=&A'\frac{\partial}{\partial t}\left(B'C'\right)+B'C'\frac{\partial A'}{\partial t}\\=&A'\left(B'\frac{\partial C'}{\partial t}+C'\frac{\partial B'}{\partial t}\right)+B'C'\frac{\partial A'}{\partial t}\\=&A'B'\frac{\partial C'}{\partial t}+A'C'\frac{\partial B'}{\partial t}+B'C'\frac{\partial A'}{\partial t}\ .\end{aligned}\tag{34}$$

Using (28), (29), and a similar equation for C', we get

$$\begin{aligned}&\rho_0\left[\frac{\partial}{\partial t}\left(A'B'C'\right)+\bar{u}_j\frac{\partial}{\partial x_j}\left(A'B'C'\right)+u'_jB'C'\frac{\partial\overline{A}}{\partial x_j}+u'_jA'C'\frac{\partial\overline{B}}{\partial x_j}+u'_jA'B'\frac{\partial\overline{C}}{\partial x_j}+u'_j\frac{\partial}{\partial x_j}\left(A'B'C'\right)\right]\\&+B'C'\frac{\partial}{\partial x_j}\left[-\rho_0\overline{u'_jA'}+\left(M'_A\right)_j\right]+A'C'\frac{\partial}{\partial x_j}\left[-\rho_0\overline{u'_jB'}+\left(M'_B\right)_j\right]+A'B'\frac{\partial}{\partial x_j}\left[-\rho_0\overline{u'_jC'}+\left(M'_C\right)_j\right]\\&=B'C'S'_A+A'C'S'_B+A'B'S'_C\ .\end{aligned}\tag{35}$$

Use of the two continuity equations (13) and (14) allows us to rewrite (35) as

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\rho_0A'B'C'\right)+\frac{\partial}{\partial x_j}\left(\rho_0\bar{u}_jA'B'C'+\rho_0u'_jA'B'C'\right)+\rho_0u'_jB'C'\frac{\partial\overline{A}}{\partial x_j}+\rho_0u'_jA'C'\frac{\partial\overline{B}}{\partial x_j}+\rho_0u'_jA'B'\frac{\partial\overline{C}}{\partial x_j}\\&+B'C'\frac{\partial}{\partial x_j}\left[-\rho_0\overline{u'_jA'}+\left(M'_A\right)_j\right]+A'C'\frac{\partial}{\partial x_j}\left[-\rho_0\overline{u'_jB'}+\left(M'_B\right)_j\right]+A'B'\frac{\partial}{\partial x_j}\left[-\rho_0\overline{u'_jC'}+\left(M'_C\right)_j\right]\\&=B'C'S'_A+A'C'S'_B+A'B'S'_C\ .\end{aligned}\tag{36}$$

Notice that we are going to have gradient-production terms again. Move those terms to the right-hand side:

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(\rho_0 A'B'C'\right)+\frac{\partial}{\partial x_j}\left(\rho_0\bar{u}_j A'B'C'+\rho_0 u'_j A'B'C'\right)\\
&+B'C'\frac{\partial}{\partial x_j}\left(M'_A\right)_j+A'C'\frac{\partial}{\partial x_j}\left(M'_B\right)_j+A'B'\frac{\partial}{\partial x_j}\left(M'_C\right)_j\\
&=B'C'\frac{\partial}{\partial x_j}\left(\rho_0\overline{u'_jA'}\right)+A'C'\frac{\partial}{\partial x_j}\left(\rho_0\overline{u'_jB'}\right)+A'B'\frac{\partial}{\partial x_j}\left(\rho_0\overline{u'_jC'}\right)\\
&-\rho_0 u'_j B'C'\frac{\partial\overline{A}}{\partial x_j}-\rho_0 u'_j A'C'\frac{\partial\overline{B}}{\partial x_j}-\rho_0 u'_j A'B'\frac{\partial\overline{C}}{\partial x_j}\\
&+B'C'S'_A+A'C'S'_B+A'B'S'_C\,.
\end{aligned}\tag{37}$$

Separate the molecular terms into the transport parts and the dissipation parts:

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(\rho_0 A'B'C'\right)+\frac{\partial}{\partial x_j}\left[\rho_0\bar{u}_j A'B'C'+\rho_0 u'_j A'B'C'+B'C'\left(M'_A\right)_j+A'C'\left(M'_B\right)_j+A'B'\left(M'_C\right)_j\right]\\
&=B'C'\frac{\partial}{\partial x_j}\left(\rho_0\overline{u'_jA'}\right)+A'C'\frac{\partial}{\partial x_j}\left(\rho_0\overline{u'_jB'}\right)+A'B'\frac{\partial}{\partial x_j}\left(\rho_0\overline{u'_jC'}\right)\\
&-\rho_0 u'_j B'C'\frac{\partial\overline{A}}{\partial x_j}-\rho_0 u'_j A'C'\frac{\partial\overline{B}}{\partial x_j}-\rho_0 u'_j A'B'\frac{\partial\overline{C}}{\partial x_j}\\
&+B'C'S'_A+A'C'S'_B+A'B'S'_C\\
&+\left(M'_A\right)_j\frac{\partial}{\partial x_j}\left(B'C'\right)+\left(M'_B\right)_j\frac{\partial}{\partial x_j}\left(A'C'\right)+\left(M'_C\right)_j\frac{\partial}{\partial x_j}\left(A'B'\right)\,.
\end{aligned}\tag{38}$$

Finally, Reynolds-average the result:

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(\rho_0\overline{A'B'C'}\right)+\frac{\partial}{\partial x_j}\left[\rho_0\bar{u}_j\overline{A'B'C'}+\rho_0\overline{u'_jA'B'C'}+\overline{B'C'(M'_A)_j}+\overline{A'C'(M'_B)_j}+\overline{A'B'(M'_C)_j}\right]\\
&=\overline{B'C'}\frac{\partial}{\partial x_j}\left(\rho_0\overline{u'_jA'}\right)+\overline{A'C'}\frac{\partial}{\partial x_j}\left(\rho_0\overline{u'_jB'}\right)+\overline{A'B'}\frac{\partial}{\partial x_j}\left(\rho_0\overline{u'_jC'}\right)\\
&-\rho_0\overline{u'_jB'C'}\frac{\partial\bar{A}}{\partial x_j}-\rho_0\overline{u'_jA'C'}\frac{\partial\bar{B}}{\partial x_j}-\rho_0\overline{u'_jA'B'}\frac{\partial\bar{C}}{\partial x_j}\\
&+\overline{B'C'S'_A}+\overline{A'C'S'_B}+\overline{A'B'S'_C}\\
&+\overline{(M'_A)_j\frac{\partial}{\partial x_j}(B'C')}+\overline{(M'_B)_j\frac{\partial}{\partial x_j}(A'C')}+\overline{(M'_C)_j\frac{\partial}{\partial x_j}(A'B')}\,.
\end{aligned} \tag{39}$$

For the special case of purely vertical transport, this reduces to

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(\rho_0\overline{A'B'C'}\right)+\frac{\partial}{\partial z}\left[\rho_0\overline{w}\overline{A'B'C'}+\rho_0\overline{w'A'B'C'}+\overline{B'C'(M'_A)_j}+\overline{A'C'(M'_B)_j}+\overline{A'B'(M'_C)_j}\right]\\
&=\overline{B'C'}\frac{\partial}{\partial z}\left(\rho_0\overline{w'A'}\right)+\overline{A'C'}\frac{\partial}{\partial z}\left(\rho_0\overline{w'B'}\right)+\overline{A'B'}\frac{\partial}{\partial z}\left(\rho_0\overline{w'C'}\right)\\
&-\rho_0\overline{w'B'C'}\frac{\partial\bar{A}}{\partial z}-\rho_0\overline{w'A'C'}\frac{\partial\bar{B}}{\partial z}-\rho_0\overline{w'A'B'}\frac{\partial\bar{C}}{\partial z}\\
&+\overline{B'C'S'_A}+\overline{A'C'S'_B}+\overline{A'B'S'_C}\\
&+\overline{(M'_A)_z\frac{\partial}{\partial z}(B'C')}+\overline{(M'_B)_z\frac{\partial}{\partial z}(A'C')}+\overline{(M'_C)_z\frac{\partial}{\partial z}(A'B')}\,.
\end{aligned} \tag{40}$$

8 Predicting the turbulent flux of potential temperature

After Reynolds-averaging, the flux form of the potential temperature equation can be written as

$$\frac{\partial}{\partial t}\left(\rho_0\bar{\theta}\right)+\frac{\partial}{\partial x_j}\left(\rho_0\bar{u}_j\bar{\theta}+\rho_0\overline{u'_j\theta'}+\bar{H}_j\right)=\frac{\theta_0}{T_0}\frac{\bar{Q}}{c_p} \tag{41}$$

which leads to the advective form

$$\rho_0\left(\frac{\partial\bar{\theta}}{\partial t}+\bar{u}_j\frac{\partial\bar{\theta}}{\partial x_j}\right)=-\frac{\partial}{\partial x_j}\left(\rho_0\overline{u_j'\theta'}\right)+\frac{\theta_0}{T_0}\frac{\bar{Q}}{c_p}-\frac{\partial\bar{H}_j}{\partial x_j}. \tag{42}$$

Subtraction of (42) from (6) gives

$$\rho_0\left(\frac{\partial\theta'}{\partial t}+\overline{u_j}\frac{\partial\theta'}{\partial x_j}+u_j'\frac{\partial\bar{\theta}}{\partial x_j}+u_j'\frac{\partial\theta'}{\partial x_j}\right)=-\frac{\partial}{\partial x_j}\left(\rho_0\overline{u_j'\theta'}\right)+\frac{\theta_0}{T_0}\frac{Q'}{c_p}-\frac{\partial H_j'}{\partial x_j} \tag{43}$$

Multiplying (43) by u_i' yields

$$\rho_0\left(u_i'\frac{\partial\theta'}{\partial t}+u_i'\overline{u_j}\frac{\partial\theta'}{\partial x_j}+u_i'u_j'\frac{\partial\bar{\theta}}{\partial x_j}+u_i'u_j'\frac{\partial\theta'}{\partial x_j}\right)=-u_i'\frac{\partial}{\partial x_j}\left(\rho_0\overline{u_j'\theta'}\right)+u_i'\frac{\theta_0}{T_0}\frac{Q'}{c_p}-u_i'\frac{\partial H_j'}{\partial x_j} \tag{44}$$

Multiplying (18) by $\rho_0\theta'$, adding the result to (44), averaging, and combining terms, we obtain a prognostic equation for the potential temperature flux, $\rho_0\overline{u_i'\theta'}$:

$$\boxed{\begin{aligned}&\frac{\partial}{\partial t}\left(\rho_0\overline{u_i'\theta'}\right)+\frac{\partial}{\partial x_j}\left(\bar{u}_j\rho_0\overline{u_i'\theta'}+\overline{u_j'\rho_0u_i'\theta'}\right)\\&=-\rho_0\overline{u_i'u_j'}\frac{\partial\bar{\theta}}{\partial x_j}-\rho_0\overline{u_j'\theta'}\frac{\partial\bar{u}_i}{\partial x_j}+2\varepsilon_{i,j,k}\rho_0\overline{u_j'\theta'}\Omega_k\\&-\rho_0\overline{\theta'\frac{\partial}{\partial x_j}\left(\frac{\delta p'}{\rho_0}\right)}+\rho_0\frac{\overline{(\theta')^2}}{\theta_0}g_i+\overline{\theta'\frac{\partial\mathscr{F}_{i,j}'}{\partial x_j}}+\frac{\theta_0}{T_0}\frac{\overline{u_i'Q'}}{c_p}-\overline{u_i'\frac{\partial H_j'}{\partial x_j}}\end{aligned}} \tag{45}$$

Again, a "triple correlation" has appeared. The components of the potential temperature flux predicted by (45) can be used in (41), (16), and (22).

Notice that (25) contains $\overline{(\theta')^2}$, which can also be predicted, using a special case of (33):

$$\boxed{\begin{aligned}&\frac{\partial}{\partial t}\left[\frac{1}{2}\rho_0\overline{(\theta')^2}\right]+\frac{\partial}{\partial x_j}\left[\bar{u}_j\frac{1}{2}\rho_0\overline{(\theta')^2}+\overline{u_j'\frac{1}{2}\rho_0(\theta')^2}+\overline{H_j'\theta'}\right]=\\&-\rho_0\overline{u_j'\theta'}\frac{\partial\bar{\theta}}{\partial x_j}+\frac{\theta_0}{T_0}\frac{\overline{\theta'Q'}}{c_p}-\overline{H_j'\frac{\partial\theta'}{\partial x_j}}.\end{aligned}} \tag{46}$$

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

The Reynolds-averaged conservation equation for total water substance is

$$\frac{\partial}{\partial t}\left(\rho_0\overline{q_t}\right)+\frac{\partial}{\partial x_j}\left(\rho_0\bar{u}_j\overline{q_t}+\rho_0\overline{u_j{}'q_t'}+\bar{W}_j\right)=\bar{S}_w, \tag{47}$$

where

$$W_j=-\kappa\frac{\partial w}{\partial x_j} \tag{48}$$

is the flux of due to molecular diffusion.

By analogy with (45), we find that

$$\boxed{\begin{aligned}&\frac{\partial}{\partial t}\left(\rho_0\overline{u_i{}'q_t'}\right)+\frac{\partial}{\partial x_j}\left(\bar{u}_j\rho_0\overline{u_i{}'q_t'}+\overline{u_j{}'\rho_0u_i{}'q_t'}\right)\\&=-\rho_0\overline{u_i{}'u_j{}'}\frac{\partial\overline{q_t}}{\partial x_j}-\rho_0\overline{u_j{}'q_t'}\frac{\partial\bar{u}}{\partial x_j}+2\varepsilon_{i,j,k}\rho_0\overline{u_j{}'q_t'}\Omega_k\\&-\overline{\rho_0q_t'\frac{\partial}{\partial x_j}\left(\frac{\delta p'}{\rho_0}\right)}+\rho_0\frac{\overline{q_t'\theta'}}{\theta_0}g_i+\overline{q_t'\frac{\partial\mathscr{F}_{i,j}'}{\partial x_j}}+\overline{u_i{}'S'_w}-\overline{u_i{}'\frac{\partial W_j'}{\partial x_j}}\;.\end{aligned}} \tag{49}$$

The buoyancy term of (49) is proportional to the covariance of q_t and θ, which can be predicted using a special case of (33):

$$\boxed{\begin{aligned}&\frac{\partial}{\partial t}\left(\rho_0\overline{q_t'\theta'}\right)+\frac{\partial}{\partial x_j}\left(\bar{u}_j\rho_0\overline{q_t'\theta'}+\overline{u_j{}'\rho_0q_t'\theta'}\right)\\&=-\rho_0\overline{u_j{}'\theta'}\frac{\partial\overline{q_t}}{\partial x_j}-\rho_0\overline{u_j{}'q_t'}\frac{\partial\bar{\theta}}{\partial x_j}+\frac{\theta_0}{c_pT_0}\overline{q_t'Q'}+\overline{\theta'S'_w}-\overline{q_t'\frac{\partial H_j'}{\partial x_j}}-\overline{\theta'\frac{\partial W_j'}{\partial x_j}}\;.\end{aligned}} \tag{50}$$

We can also use (33) to write a prediction equation for $\overline{q_t'^2}$. Although this quantity does not appear in any of our other equations, it may be useful to know for other purposes, e.g., to determine the fractional cloudiness following methods like those of Sommeria and Deardorff (1977). We include the equation for completeness:

$$\boxed{\begin{aligned}&\frac{\partial}{\partial t}\left[\frac{1}{2}\rho_0\overline{(q_t')^2}\right]+\frac{\partial}{\partial x_j}\left[\bar{u}_j\frac{1}{2}\rho_0\overline{(q_t')^2}+\overline{u_j{}'\frac{1}{2}\rho_0(q_t')^2}+\overline{q_t'W_j'}\right]\\&=-\rho_0\overline{u_j{}'q_t'}\frac{\partial\overline{q_t}}{\partial x_j}+\overline{q_t'S'_w}+\overline{W_j'\frac{\partial q_t'}{\partial x_j}}\end{aligned}} \tag{51}$$

9 Discussion

The second- and third-moment equations are satisfied if all primed quantities vanish. In that sense, the equations do not explain *why* the flow is turbulent; they only state that certain interrelationships must be satisfied by any disturbances that arise. The explanation for the existence of turbulence is usually given in terms of instabilities, especially shearing instability.

It is also important to realize that the "fluctuations" described by the second- and third-moment equations need not necessarily be turbulent in any sense. For example, they may be orderly wave motions. They can be used to describe ensembles of cumulus clouds, mesoscale convection, and even (with a change of coordinate systems and other minor adjustments) the effects of large-scale zonally asymmetric motions on the zonally-averaged global circulation of the atmosphere.

"Realizability" is an issue that arises in the use of these equations. For example, the equations might predict a negative variance, which is impossible. We say that a negative variance is "not realizable." As a second example, is mathematically necessary. As discussed later, similar conditions can be derived for the third moments.

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 four types: triple moments, second and higher moments involving pressure fluctuations, second and higher moments involving molecular fluxes, and second and higher moments involving source-sink terms.

10 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 used to parameterize cumulus convection.

As noted above, the problem with this approach is that the second-moment equations involve unknown quantities. These terms have to be "modeled" or "parameterized," in terms of known quantities.

Donaldson (1973) gave a very readable introduction to the use of the prediction equations for the second moments. He listed four principles that, he argued, should be applied in devising parameterizations of the terms of the second-moment equations:

- A parameterization must have the same dimensions as the term it replaces. There is no room for *dimensional* numerical parameters.
- A parameterization must satisfy all the conservation relationships known to govern the variables in question. For example, a transport term must integrate to zero over the domain (in the absence of boundary fluxes).
- A parameterization must have all the tensor properties and all the symmetries of the term that it replaces.
- A parameterization must be invariant under a Galilean transformation, i.e., if we shift to a second coordinate system that is in constant motion relative to the first, the equations must be unchanged.

All authors mentioned here use the "tendency-towards-isotropy" model of the pressure-shear covariance terms of the Reynolds stress equation, which is

$$\begin{aligned}\frac{\partial}{\partial t}\left(\rho_0\overline{u_i'u_l'}\right) \sim & \overline{\frac{\delta p'}{\rho_0}\left[\frac{\partial}{\partial x_i}\left(\rho_0 u_l'\right)+\frac{\partial}{\partial x_l}\left(\rho_0 u_i'\right)\right]} \\ & = -\left(\frac{\rho_0 q}{3l_1}\right)\left(\overline{u_i'u_l'}-\frac{\delta_{i,l}}{3}q^2\right),\end{aligned} \tag{52}$$

where

$$\begin{aligned}q^2 \equiv & \overline{u_k'u_k'} \\ \equiv & 2e\ ,\end{aligned} \tag{53}$$

and l_1 is a length scale that has to be supplied as part of the parameterization. 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 $q^2/3$, so that $\overline{u_i' u_l'} - \frac{\delta_{i,l}}{3} q^2$, which appears on the right-hand-side of (52), will vanish. The term is thus formulated as a measure of the departure from isotropy. If $\overline{u_i' u_l'}$ departs from its "isotropic value" (0 for the off-diagonal members, and $q^2/3$ 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

$$\overline{p' \frac{\partial \theta'}{\partial x_i}} = -\frac{q}{3 l_2} \left(\overline{u_i' \theta'} \right) \tag{54}$$

and

$$\overline{p' \frac{\partial q_t'}{\partial x_i}} = -\frac{q}{3 l_3} \left(\overline{u_i' q_t'} \right) \tag{55}$$

in the prediction equations for $\rho_0 \overline{u_i' \theta'}$ and $\rho_0 \overline{u_i' q_t'}$ respectively. These formulations tend to damp the fluxes towards zero.

The remaining pressure terms of these equations are all derivatives, and so should tend to vanish when integrated over sufficiently large regions. They are often parameterized as diffusion terms, in which the "fluxes" are given as follows:

$$\overline{p' u'_k} = -\rho_0 \lambda_1 q \frac{\partial}{\partial x_i} \left(\overline{u_i' u'_k} \right), \tag{56}$$

$$\overline{p' \theta'} = -\rho_0 \lambda_1 q \frac{\partial}{\partial x_i} \left(\overline{u_i' \theta'} \right), \tag{57}$$

$$\overline{p' q_t'} = -\rho_0 \lambda_1 q \frac{\partial}{\partial x_i} \left(\overline{u_i' q_t'} \right). \tag{58}$$

The "triple correlation" terms of the second-moment equations are also transport terms, and are sometimes parameterized as diffusion. The complete model is then

$$
\begin{aligned}
&-\frac{\partial}{\partial x_j}\left(\rho_0\overline{u'_i u'_j u'_l}\right)-\frac{\partial}{\partial x_i}\left(\overline{u'_l p'}\right)-\frac{\partial}{\partial x_l}\left(\overline{u'_i p'}\right) \\
&=\frac{\partial}{\partial x_k}\left\{q\lambda_1\left[\frac{\partial}{\partial x_k}\left(\rho_0\overline{u'_i u'_l}\right)+\frac{\partial}{\partial x_i}\left(\rho_0\overline{u'_l u'_k}\right)+\frac{\partial}{\partial x_l}\left(\rho_0\overline{u'_k u'_i}\right)\right]\right\},
\end{aligned}
\tag{59}
$$

$$
-\frac{\partial}{\partial x_j}\left(\overline{u'_j\rho_0 u'_i w'}\right)-\rho_0\frac{\partial}{\partial x_i}\left(\frac{\overline{p'w'}}{\rho_0}\right)=\frac{\partial}{\partial x_k}\left\{q\lambda_4\left[\frac{\partial}{\partial x_k}\left(\rho_0\overline{u'_i w'}\right)+\frac{\partial}{\partial x_i}\left(\rho_0\overline{u'_i w'}\right)\right]\right\}. \tag{60}
$$

Similarly, the triple correlation terms of the scalar variance and covariance forecast equations can be parameterized as down-gradient diffusion terms:

$$
-\frac{\partial}{\partial x_j}\left(\overline{u'_j\frac{1}{2}\rho_0(\theta')^2}\right)=\frac{\partial}{\partial x_k}\left\{q\lambda_2\frac{\partial}{\partial x_k}\left[\frac{1}{2}\rho_0\overline{(\theta')^2}\right]\right\}, \tag{61}
$$

$$
-\frac{\partial}{\partial x_j}\left(\overline{u'_j\rho_0 q'_t\theta'}\right)=\frac{\partial}{\partial x_k}\left[q\lambda_5\frac{\partial}{\partial x_k}\left(\rho_0\overline{q'_t\theta'}\right)\right], \tag{62}
$$

$$
-\frac{\partial}{\partial x_j}\left(\overline{u'_j\frac{1}{2}\rho_0(q'_t)^2}\right)=\frac{\partial}{\partial x_k}\left\{q\lambda_6\frac{\partial}{\partial x_k}\left[\frac{1}{2}\rho_0\overline{(q'_t)^2}\right]\right\}. \tag{63}
$$

All of these assumptions are “safe” in the sense that the parameterizations will not blow up in a computer simulation. None of the assumptions is very convincing, but there is what Lumley calls an “article of faith,” which is that weak assumptions at third order are preferable to weak assumptions at second order (Lumley and Khajeh-Nouri 1975; Wyngaard 1975).

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

$$
-\frac{\overline{\mathscr{F}'_{i,j}}}{\rho_0}\frac{\partial u'_l}{\partial x_j}-\frac{\overline{\mathscr{F}'_{l,j}}}{\rho_0}\frac{\partial u'_i}{\partial x_j}=-\frac{2}{3}\frac{q^3}{\Lambda_1}\delta_{i,l}, \tag{64}
$$

$$
\frac{\partial}{\partial x_j}\left(\overline{u'_l\mathscr{F}'_{i,j}}+\overline{u'_i\mathscr{F}'_{l,j}}\right)=0, \tag{65}
$$

$$\overline{\theta' \frac{\partial \mathscr{F}'_{i,j}}{\partial x_j}} - \overline{u'_i \frac{\partial H'_j}{\partial x_j}} = 0, \tag{66}$$

$$\overline{H'_j \frac{\partial \theta'}{\partial x_j}} = -\frac{2q}{\Lambda_2} \overline{(\theta')^2}, \tag{67}$$

$$-\frac{\partial}{\partial x_j} \overline{\left(H'_j \theta' \right)} = 0, \tag{68}$$

$$\overline{-u'_i \frac{\partial W'_j}{\partial x_j}} = 0, \tag{69}$$

$$-\overline{q'_t \frac{\partial H'_j}{\partial x_j}} - \overline{\theta' \frac{\partial W'_j}{\partial x_j}} = 0, \tag{70}$$

$$-\overline{W'_j \frac{\partial q'_t}{\partial x_j}} = \frac{2q}{\Lambda_3} \overline{(q'_t)^2}, \tag{71}$$

$$-\frac{\partial}{\partial x_j} \overline{\left(W'_j q'_t \right)} = 0. \tag{72}$$

The heating and moistening terms are usually ignored:

$$\frac{\theta_0}{T_0} \frac{\overline{u'_i Q'}}{c_p} = 0, \tag{73}$$

$$\frac{\theta_0}{T_0} \frac{\overline{\theta' Q'}}{c_p} = 0, \tag{74}$$

$$\overline{u'_i S'_{qt}} = 0, \tag{75}$$

$$\frac{\theta_0}{T_0} \frac{\overline{q'_t Q'}}{c_p} + \overline{\theta' S'_{qt}} = 0, \tag{76}$$

$$\overline{q'_t S'_{qt}} = 0. \tag{77}$$

Their potential importance must be faced, however, where the equations are applied to clouds. The problem can be greatly simplified by predicting moist conservative variables (e.g, equivalent potential temperature) instead of dry conservative variables (e.g., potential temperature).

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 tacitly assumed that they are.

Mellor and Yamada (1974) presented a hierarchy of turbulence closure models, ranging form a fully prognostic system of second-moment equations (Level 4) to a fully diagnostic subset corresponding to mixing length theory (Level 1). They attempt to justify the hierarchies using expansions in terms of small parameters, but I don?t find the argument very convincing.

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 production of momentum, heat, and moisture fluxes. All of the models are Boussinesq.

- Level 4 includes a total of 15 prognostic 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 prognostic equations are used for the second moments - those for e, $\overline{(\theta')^2}$, and $\overline{(q_t')^2}$.
- 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, relative to Level 3, was not sufficient to warrant the additional complexity. Of course, this conclusion was based in part on the parameterizations that they used for the triple moments, the dissipation terms, and the pressure terms.

11 The third-moment equations

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

$$\frac{\partial w'^3}{\partial t} = 3w'^2 \frac{\partial w'}{\partial t}. \tag{78}$$

Here $w' \equiv u'_3$; in the following, we also use $z \equiv x_3$, and we replace g_i by g. From (18) we find that

$$\begin{aligned} &\frac{\partial w'}{\partial t} + \bar{u}_j \frac{\partial w'}{\partial x_j} + u'_j \frac{\partial \bar{w}}{\partial x_j} + u'_j \frac{\partial w'}{\partial x_j} \\ &= 2\varepsilon_{3,j,k} u'_j \Omega_k - \frac{\partial}{\partial z}\left(\frac{\delta p'}{\rho_0}\right) + \frac{\delta\theta'}{\theta_0} g + \frac{1}{\rho_0}\frac{\partial}{\partial x_i}\left(\mathscr{F}'_{3,j} - \rho_0 \overline{w'u'_j}\right). \end{aligned} \tag{79}$$

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

$$\begin{aligned} &\frac{\partial}{\partial t} w'w'w' + \bar{u}_j \frac{\partial}{\partial x_j} w'w'w' + 3w'w'u'_j \frac{\partial \bar{w}}{\partial x_j} + u'_j \frac{\partial}{\partial x_j} w'w'w' \\ &= 6\varepsilon_{3,j,k} u'_j w'w' \Omega_k - 3w'w' \frac{\partial}{\partial z}\left(\frac{\delta p'}{\rho_0}\right) + 3\frac{g}{\theta_0} w'w'\delta\theta' + \frac{3w'w'}{\rho_0}\frac{\partial}{\partial x_j}\left(\mathscr{F}'_{3,j} - \rho_0 \overline{w'u'_j}\right). \end{aligned} \tag{80}$$

Use of the continuity equation for the fluctuating part of the flow, and averaging, introduces a "fourth moment" term. The final result is

$$\boxed{\begin{aligned} &\frac{\partial}{\partial t}\overline{w'w'w'} + \bar{u}_j \frac{\partial}{\partial x_j}\overline{w'w'w'} + 3\overline{w'w'u'_j}\frac{\partial \bar{w}}{\partial x_j} + \frac{1}{\rho_0}\frac{\partial}{\partial x_j}\left(\rho_0 \overline{u'_j w'w'w'}\right) = \\ &6\varepsilon_{3,j,k}\overline{u'_j w'w'}\Omega_k - 3\overline{w'w'\frac{\partial}{\partial z}\left(\frac{\delta p'}{\rho_0}\right)} + 3\frac{g_i}{\theta_0}\overline{w'w'\delta\theta'} + \frac{3}{\rho_0}\overline{w'w'\frac{\partial \mathscr{F}'_{3,j}}{\partial x_j}} - \frac{3\overline{w'w'}}{\rho_0}\frac{\partial}{\partial x_j}\left(\rho_0 \overline{w'u'_j}\right) \end{aligned}}\ . \tag{81}$$

Normally (81) is simplified by neglecting advection by the mean flow, the production term involving $\frac{\partial \bar{w}}{\partial x_j}$, the rotation term, and $\frac{3\overline{w'w'}}{\rho_0}\frac{\partial}{\partial x_j}\left(\rho_0 \overline{w'u'_j}\right)$:

An equation to predict $\overline{\theta'\theta'\theta'}$ can be written down by mimicking (39), with reference to (6):

$$\boxed{\begin{aligned}&\frac{\partial}{\partial t}\overline{\theta'\theta'\theta'}+\bar{u}_j\frac{\partial}{\partial x_j}\overline{\theta'\theta'\theta'}+3\overline{w'w'u'_j}\frac{\partial\overline{\theta}}{\partial x_j}+\frac{1}{\rho_0}\frac{\partial}{\partial x_j}\left(\rho_0\overline{u'_j\theta'\theta'\theta'}\right)=\\&\frac{3}{\rho_0}\overline{\theta'\theta'\frac{\partial H'_j}{\partial x_j}}-\frac{3\overline{\theta'\theta'}}{\rho_0}\frac{\partial}{\partial x_j}\left(\rho_0\overline{u'_j\theta'}\right).\end{aligned}} \tag{82}$$

12 Third-order closure

Jean Claude André and collaborators (André et al. 1976a,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 assumption":

$$\overline{a'b'c'd'} \cong \overline{a'b'}\;\overline{c'd'}+\overline{a'c'}\;\overline{b'd'}+\overline{a'd'}\;\overline{b'c'}, \tag{83}$$

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

$$\left|\overline{a'b'c'}\right| \le \min\left\{\sqrt{a^2\left[\overline{b^2}\overline{c'^2}+\left(\overline{b'c'}\right)^2\right]}\,,\sqrt{b^2\left[\overline{a^2}\overline{c'^2}+\left(\overline{a'c'}\right)^2\right]}\,,\sqrt{c^2\left[\overline{a^2}\overline{b'^2}+\left(\overline{a'b'}\right)^2\right]}\right\}. \tag{84}$$

This is an example of a "realizability" constraint.

Krueger (1988) used third-moment closure in a cloud-resolving model.

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References

André, J., G. De Moor, P. Lacarrere, and R. Du Vachat, 1976a: Turbulence approximation for inhomogeneous flows: Part I. The clipping approximation. *Journal of the Atmospheric Sciences*, **33 (3)**, 476–481.

André, J., G. De Moor, P. Lacarrere, and R. Du Vachat, 1976b: Turbulence approximation for inhomogeneous flows: Part II. The numerical simulation of a penetrative convection experiment. *Journal of the Atmospheric Sciences*, **33 (3)**, 482–491.

André, J., G. De Moor, P. Lacarrere, and R. Du Vachat, 1978: Modeling the 24-hour evolution of the mean and turbulent structures of the planetary boundary layer. *Journal of the Atmospheric Sciences*, **35 (10)**, 1861–1883.

Donaldson, C., 1973: Construction of a dynamic model of the production of atmospheric turbulence and the dispersal of atmospheric pollutants. *Workshop on Micrometeorology*, N. Busch, D. Haugen, and A. M. Society, Eds., American Meteorological Society.

Krueger, S. K., 1988: Numerical simulation of tropical cumulus clouds and their interaction with the subcloud layer. *Journal of the atmospheric sciences*, **45 (16)**, 2221–2250.

Lumley, J. L., and B. Khajeh-Nouri, 1975: Computational modeling of turbulent transport. *Advances in Geophysics*, Vol. 18, Elsevier, 169–192.

Mellor, G. L., and T. Yamada, 1974: A hierarchy of turbulence closure models for planetary boundary layers. *Journal of the Atmospheric Sciences*, **31 (7)**, 1791–1806.

Rotta, J., 1951: Statistische theorie nichthomogener turbulenz. *Zeitschrift für Physik*, **129 (6)**, 547–572.

Sommeria, G., and J. Deardorff, 1977: Subgrid-scale condensation in models of nonprecipitating clouds. *Journal of the Atmospheric Sciences*, **34 (2)**, 344–355.

Wyngaard, J. C., 1975: Modeling the planetary boundary layer—extension to the stable case. *Boundary-Layer Meteorology*, **9 (4)**, 441–460.