

## The continuity and thermodynamic energy equations

**T**HE continuity equations for air, individual gases, and aerosol particles, and the thermodynamic energy equation are fundamental equations in atmospheric models. Continuity equations are used to simulate changes in concentration or mixing ratio of a variable over time and take account of transport, external sources, and external sinks of the variable. The thermodynamic energy equation is used to predict changes in temperature with time and takes account of transport, external sources, and external sinks of energy. In this chapter, scalars, vectors, gradient operators, local derivatives, and total derivatives are defined, and the continuity and thermodynamic energy equations are derived.

### 3.1 DEFINITIONS

In this section, definitions relating to wind speed and direction and differentiation are provided. The definitions will be used in subsequent sections to derive time-dependent continuity equations.

#### 3.1.1 Wind velocity

**Scalars** are variables, such as temperature, air pressure, and air mass, that have magnitude but not direction. **Vectors** are variables, such as velocity, that have magnitude and direction.

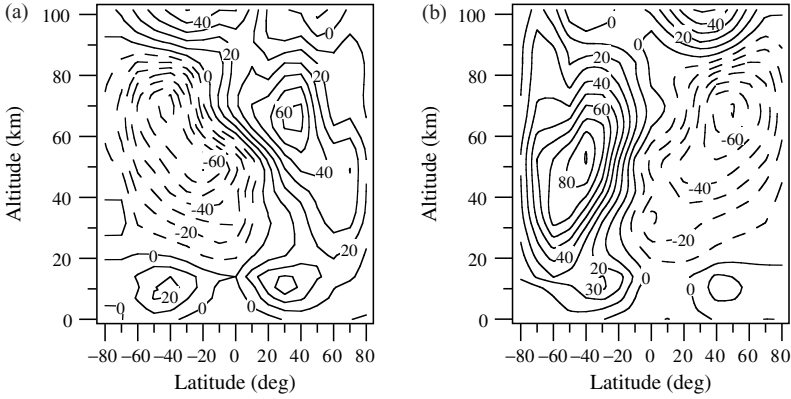
Winds are described by three parameters – velocity, the scalar components of velocity, and speed. **Velocity** is a vector that quantifies the rate at which the position of a body changes over time. Total and horizontal wind velocity vectors are defined in Cartesian (rectangular) horizontal coordinates as

$$\mathbf{v} = iu + jv + kw \quad \mathbf{v}_h = iu + jv \quad (3.1)$$

respectively, where  $\mathbf{i}$ ,  $\mathbf{j}$ , and  $\mathbf{k}$  are Cartesian-coordinate west–east, south–north, and vertical unit vectors, respectively, and

$$u = \frac{dx}{dt} \quad v = \frac{dy}{dt} \quad w = \frac{dz}{dt} \quad (3.2)$$

are scalar components of velocity (**scalar velocities**) ( $\text{m s}^{-1}$ ). Scalar velocities have magnitude only. When applied in (3.1), positive  $u$ ,  $v$ , and  $w$  correspond to winds



**Figure 3.1** Zonally averaged west–east scalar velocities ( $\text{m s}^{-1}$ ) for (a) January and (b) July. Data for the plots were compiled by Fleming *et al.* (1988).

moving from west to east, south to north, and lower to higher elevation, respectively. The vertical scalar velocity in (3.2) is written in the **altitude vertical coordinate** system. In this coordinate system (coordinate), tops and bottoms of horizontal layers are defined by surfaces of constant altitude.

The magnitude of the wind is its speed. The total and horizontal wind speeds are defined as

$$|\mathbf{v}| = \sqrt{u^2 + v^2 + w^2} \quad |\mathbf{v}_h| = \sqrt{u^2 + v^2} \quad (3.3)$$

respectively.

Wind **direction** is generally named for where a wind originates from. A westerly wind, southwesterly wind, sea breeze, and mountain breeze originate from the west, the southwest, the sea, and a mountain, respectively. A positive scalar velocity  $u$  with no south–north component is a westerly wind. A positive scalar velocity  $v$  with no west–east component is a southerly wind.

Air velocities vary in space and time. Figures 3.1(a) and (b) show global-scale latitude–altitude contour plots of zonally averaged west–east scalar velocities for January and July, respectively. The figures indicate that west–east winds in the upper troposphere almost always originate from the west. The two peaks near 10 km in each figure correspond to **subtropical jet streams**. Near the surface at the Equator and poles, winds originate from the east but are weak. Near the surface at midlatitudes ( $30^\circ$ – $60^\circ$ ) in both hemispheres, winds originate from the west. In the stratosphere, westerly wind speeds increase with height in the winter hemisphere (Northern Hemisphere in January; Southern Hemisphere in July), forming **polar night jets** near 60 km. Easterly wind speeds increase with increasing altitude in the summer hemisphere. Winds above the surface are driven by pressure gradients, and pressure gradients are driven by temperature gradients. Thus, strong winds aloft indicate strong temperature and pressure gradients.

### 3.1 Definitions

#### 3.1.2 Time and spatial rates of change

The time rate of change of a variable, such as concentration, momentum, or temperature, can be determined at a fixed location or in the frame of reference of the variable as it moves. Suppose a plume, carrying a gas with number concentration  $N = N(t, x[t])$  (molec.  $\text{cm}^{-3}$ ), travels with the wind from fixed point A in the west to fixed point B in the east. The time rate of change of  $N$  anywhere along the plume's trajectory is the **total derivative**,  $dN/dt$ . The total derivative can be expanded with the chain rule in Cartesian coordinates as

$$\frac{dN}{dt} = \frac{\partial N}{\partial t} \frac{dt}{dt} + \frac{\partial N}{\partial x} \frac{dx}{dt} = \frac{\partial N}{\partial t} + u \frac{\partial N}{\partial x} \quad (3.4)$$

where  $\partial N/\partial t$  is the time rate of change of concentration at fixed point A (**local derivative**), and  $u\partial N/\partial x$  is the time rate of change of concentration in the plume that results from a west–east scalar velocity transporting the plume.

The total derivative of a variable is nonzero when processes other than transport affect the variable. In the case of gases, external processes include chemistry and gas-to-particle conversion. If  $dN/dt = 0$ , the concentration of a gas does not change as it travels with the wind.

The local derivative of a variable is the difference between the total derivative and the rate of change of the variable due to transport. Thus, the local derivative is affected by external processes plus transport. If  $\partial N/\partial t = 0$ , the rate of production (loss) of a variable due to external processes equals the rate of loss (production) of the variable due to transport of a spatial gradient of the variable [ $u(\partial N/\partial x)$ ].

#### Example 3.1

Suppose the time rate of change of concentration of a gas along the path of a hot-air balloon traveling with the wind from east to west at  $u = -10 \text{ m s}^{-1}$  is  $dN/dt = 10^8 \text{ molec. cm}^{-3} \text{ s}^{-1}$ . If the west–east gradient in concentration is  $\partial N/\partial x = 10^{10} \text{ molec. cm}^{-3} \text{ km}^{-1}$  (concentration increases from west to east), determine the time rate of change of concentration at a fixed point A, which the balloon passes over.

#### SOLUTION

Since  $u\partial N/\partial x = -10^8 \text{ molec. cm}^{-3} \text{ s}^{-1}$ , (3.4) predicts  $(\partial N/\partial t)_A \approx 2 \times 10^8 \text{ molec. cm}^{-3} \text{ s}^{-1}$ . Thus, transport from the east ( $u\partial N/\partial x$ ) accounts for one-half of the production rate of  $N$  at point A, and transformations along the trajectory ( $dN/dt$ ) account for the other half.

A **Lagrangian** frame of reference is a frame of reference that moves relative to a fixed coordinate system. An **Eulerian** frame of reference is a frame of reference in a fixed coordinate system. The left side of (3.4) is written in terms of a Lagrangian

frame of reference. The right side is written in terms of an Eulerian frame of reference. Generalizing (3.4) to three dimensions gives

$$\frac{dN}{dt} = \frac{\partial N}{\partial t} + u \frac{\partial N}{\partial x} + v \frac{\partial N}{\partial y} + w \frac{\partial N}{\partial z} \quad (3.5)$$

### 3.1.3 Gradient operator

A gradient operator (also called a directional derivative, nabla operator, or del operator) is a vector operator of partial derivatives. The **gradient operator in Cartesian-altitude coordinates** is

$$\nabla = \mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z} \quad (3.6)$$

The **dot product** of the velocity vector with the gradient operator is a scalar operator,

$$\mathbf{v} \cdot \nabla = (iu + jv + kw) \cdot \left( \mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z} \right) = u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} + w \frac{\partial}{\partial z} \quad (3.7)$$

where  $\mathbf{i} \cdot \mathbf{i} = 1$ ,  $\mathbf{j} \cdot \mathbf{j} = 1$ , and  $\mathbf{k} \cdot \mathbf{k} = 1$ . Cross terms are zero ( $\mathbf{i} \cdot \mathbf{j} = 0$ ,  $\mathbf{i} \cdot \mathbf{k} = 0$ , and  $\mathbf{j} \cdot \mathbf{k} = 0$ ), since the unit vectors are orthogonal. The dot product of two vectors is a scalar and symmetric (e.g.,  $\mathbf{a} \cdot \mathbf{v} = \mathbf{v} \cdot \mathbf{a}$ ). The dot product of a gradient operator with a vector is a scalar operator but not symmetric ( $\nabla \cdot \mathbf{v} \neq \mathbf{v} \cdot \nabla$ ). Instead,

$$\nabla \cdot \mathbf{v} = \left( \mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z} \right) \cdot (iu + jv + kw) = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \quad (3.8)$$

which is a scalar **divergence**. When concentration is multiplied by a divergence, the result is the scalar

$$N(\nabla \cdot \mathbf{v}) = N \frac{\partial u}{\partial x} + N \frac{\partial v}{\partial y} + N \frac{\partial w}{\partial z} \quad (3.9)$$

The gradient of a scalar, such as concentration, is a vector. For example,

$$\nabla N = \left( \mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z} \right) N = \mathbf{i} \frac{\partial N}{\partial x} + \mathbf{j} \frac{\partial N}{\partial y} + \mathbf{k} \frac{\partial N}{\partial z} \quad (3.10)$$

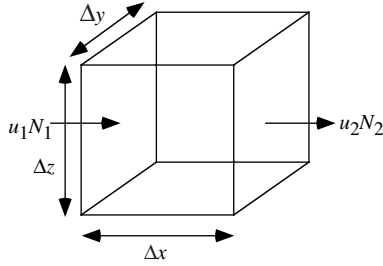
Applying the dot product of velocity with the gradient operator to  $N$  gives the scalar

$$(\mathbf{v} \cdot \nabla)N = \left( u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} + w \frac{\partial}{\partial z} \right) N = u \frac{\partial N}{\partial x} + v \frac{\partial N}{\partial y} + w \frac{\partial N}{\partial z} \quad (3.11)$$

Substituting this result into the total-derivative equation (3.5) yields

$$\frac{dN}{dt} = \frac{\partial N}{\partial t} + (\mathbf{v} \cdot \nabla)N \quad (3.12)$$

### 3.2 Continuity equations



**Figure 3.2** Example of mass conservation. The number of molecules entering minus the number of molecules leaving the box equals the number of molecules accumulating in the box.

Generalizing (3.12) for any variable gives the **total derivative in Cartesian-altitude coordinates** as

$$\frac{d}{dt} = \frac{\partial}{\partial t} + u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} + w \frac{\partial}{\partial z} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \quad (3.13)$$

### 3.2 CONTINUITY EQUATIONS

When air circulates in an enclosed volume, and no chemical or physical processes affect it, the mass of the air, summed throughout the volume, is conserved. In an atmospheric model divided into many **grid cells (grid boxes)**, the mass of air entering one cell minus the mass leaving the cell equals the final mass minus the initial mass in the cell. The same is true for other atmospheric variables, such as gas concentrations or energy, when only transport affects these variables.

Figure 3.2 shows a grid cell with dimensions  $\Delta x$ ,  $\Delta y$ ,  $\Delta z$  (m). The west–east scalar velocities entering and leaving the cell are  $u_1$  and  $u_2$  ( $\text{m s}^{-1}$ ), respectively. Gas concentrations at the west and east boundaries of the cell are  $N_1$  and  $N_2$  ( $\text{molec. cm}^{-3}$ ), respectively. Mass fluxes of gas into the cell and out of the cell are  $u_1 N_1$  and  $u_2 N_2$  ( $\text{m molec. cm}^{-3} \text{ s}^{-1}$ ), respectively.

From the information given, the numbers of molecules entering, leaving, and accumulating in the box during time period  $\Delta t$  are  $u_1 N_1 \Delta y \Delta z \Delta t$ ,  $u_2 N_2 \Delta y \Delta z \Delta t$ , and

$$\Delta N \Delta x \Delta y \Delta z = u_1 N_1 \Delta y \Delta z \Delta t - u_2 N_2 \Delta y \Delta z \Delta t \quad (3.14)$$

respectively. Dividing both sides of (3.14) by  $\Delta t$  and by the box volume ( $\Delta x \Delta y \Delta z$ ) gives

$$\frac{\Delta N}{\Delta t} = - \left( \frac{u_2 N_2 - u_1 N_1}{\Delta x} \right) \quad (3.15)$$

As  $\Delta x \rightarrow 0$  and  $\Delta t \rightarrow 0$ , this equation approaches

$$\frac{\partial N}{\partial t} = -\frac{\partial (uN)}{\partial x} \quad (3.16)$$

which is the **continuity equation** for a gas affected by velocity in one direction. This equation expands to three dimensions in Cartesian-altitude coordinates as

$\frac{\partial N}{\partial t} = -\frac{\partial (uN)}{\partial x} - \frac{\partial (vN)}{\partial y} - \frac{\partial (wN)}{\partial z} = -\nabla \cdot (\mathbf{v}N) \quad (3.17)$
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where  $\mathbf{v}N = iuN + jvN + kwN$ . A similar equation can be written for air density. Equation (3.17) states that the time rate of change of  $N$  at a fixed location equals the negative of the local spatial gradient of the flux of  $N$ . Equation (3.17) is a **flux divergence form** of the continuity equation so called because  $\nabla \cdot (\mathbf{v}N)$  is a divergence of concentration.

Substituting

$$\nabla \cdot (\mathbf{v}N) = N(\nabla \cdot \mathbf{v}) + (\mathbf{v} \cdot \nabla)N \quad (3.18)$$

into (3.17) and writing a similar equation for air density give the continuity equations for gas number concentration and total air mass density as

$$\frac{\partial N}{\partial t} = -N(\nabla \cdot \mathbf{v}) - (\mathbf{v} \cdot \nabla)N \quad (3.19)$$

$$\frac{\partial \rho_a}{\partial t} = -\rho_a(\nabla \cdot \mathbf{v}) - (\mathbf{v} \cdot \nabla)\rho_a \quad (3.20)$$

respectively. Substituting

$$(\mathbf{v} \cdot \nabla)N = \frac{dN}{dt} - \frac{\partial N}{\partial t} \quad (3.21)$$

from (3.12) into (3.19) and (3.20) gives **velocity divergence forms** of the continuity equations as

$$\frac{dN}{dt} = -N(\nabla \cdot \mathbf{v}) \quad (3.22)$$

$$\frac{d\rho_a}{dt} = -\rho_a(\nabla \cdot \mathbf{v}) \quad (3.23)$$

where  $\nabla \cdot \mathbf{v}$  is the divergence of velocity. The equations are also **advective forms** of the continuity equation in that  $d/dt$  contains the advection term,  $\mathbf{v} \cdot \nabla$ . The equations state that the change of a scalar variable over time in a moving parcel equals the scalar variable multiplied by the negative local spatial gradient of velocity.

The gas number concentration  $N$  (molecules per cubic centimeter of air) is related to the moist-air mass mixing ratio,  $q$  (kilograms per kilogram of moist air), of a

### 3.2 Continuity equations

species with molecular weight  $m$  ( $\text{g mol}^{-1}$ ) by

$$N = \frac{A\rho_a q}{m} \quad (3.24)$$

where  $A$  is Avogadro's number ( $\text{molec. mol}^{-1}$ ). Substituting (3.24) into (3.19) and expanding give

$$q \left( \frac{\partial \rho_a}{\partial t} + \rho_a (\nabla \cdot \mathbf{v}) + (\mathbf{v} \cdot \nabla) \rho_a \right) + \rho_a \frac{\partial q}{\partial t} = -\rho_a (\mathbf{v} \cdot \nabla) q \quad (3.25)$$

Substituting the continuity equation for air from (3.20) into (3.25) gives the **gas continuity equation** in units of the moist-air mass mixing ratio as

$$\frac{\partial q}{\partial t} = -(\mathbf{v} \cdot \nabla) q \quad (3.26)$$

Equations (3.22) and (3.23) assume that air is **compressible**, meaning that total volume of a parcel of air changes over time. Ocean water is considered **incompressible**, meaning that the total volume of a parcel of ocean water does not change over time. Thus,

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \quad (3.27)$$

which is the **continuity equation for an incompressible fluid**. If (3.27) is not satisfied, a net divergence out of or convergence into a fluid volume occurs, causing the volume to expand or contract, respectively. Equation (3.27) states that an **incompressible fluid is nondivergent**. The equation can also be written as  $\nabla \cdot \mathbf{v} = 0$ . Substituting water density ( $\rho_w$ ) for air density and substituting  $\nabla \cdot \mathbf{v} = 0$  into (3.23) give

$$\frac{d\rho_w}{dt} = 0 \quad (3.28)$$

which states that the density of an incompressible fluid is constant along the motion of the fluid. At a fixed point in the fluid, the density may change. Substituting water density for air density and  $\nabla \cdot \mathbf{v} = 0$  into (3.20) give

$$\frac{\partial \rho_w}{\partial t} = -(\mathbf{v} \cdot \nabla) \rho_w \quad (3.29)$$

which states that the change in water density at a fixed point in an incompressible fluid is the negative product of velocity and the spatial gradient of density. In sum, the density of an incompressible fluid, such as liquid water, can vary spatially, but the total volume of such a fluid is constant over time. A fluid in which density varies spatially throughout the fluid is **inhomogeneous**. Ocean water is inhomogeneous and incompressible. A fluid in which density is always constant throughout a volume ( $\partial \rho_w / \partial t = 0$ ) is **homogeneous**. Pure liquid water is a relatively homogeneous, incompressible fluid. **Air is an inhomogeneous and compressible fluid.**

### 3.3 EXPANDED CONTINUITY EQUATIONS

Equation (3.17) gave the continuity equation without molecular diffusion or external source and sink terms. A more complete form of the **continuity equation for a gas** is

$$\frac{\partial N}{\partial t} = -\nabla \cdot (\mathbf{v}N) + D\nabla^2 N + \sum_{n=1}^{N_{e,t}} R_n \quad (3.30)$$

(e.g., Reynolds *et al.* 1973), where  $D$  is the **molecular diffusion coefficient** of the gas ( $\text{cm}^2 \text{s}^{-1}$ ),  $N_{e,t}$  is the number of external processes (e.g., chemistry, emission, etc.) affecting the gas, and  $R_n$  is the time rate of change of trace-gas concentration due to the  $n$ th external process affecting the gas ( $\text{molec. cm}^{-3} \text{s}^{-1}$ ). **Molecular diffusion** is the movement of molecules due to their kinetic energy. As molecules move, they collide with other molecules and are redirected along arbitrary paths. A molecular diffusion coefficient quantifies the rate of molecular diffusion, and is defined mathematically in Section 16.2.

The squared gradient in the molecular diffusion term of (3.30) expands to

$$\begin{aligned} \nabla^2 N &= (\nabla \cdot \nabla) N = \left[ \left( \mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z} \right) \cdot \left( \mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z} \right) \right] N \\ &= \frac{\partial^2 N}{\partial x^2} + \frac{\partial^2 N}{\partial y^2} + \frac{\partial^2 N}{\partial z^2} \end{aligned} \quad (3.31)$$

Substituting (3.17) and (3.31) into (3.30) gives the continuity equation for a gas as

$$\frac{\partial N}{\partial t} + \frac{\partial(uN)}{\partial x} + \frac{\partial(vN)}{\partial y} + \frac{\partial(wN)}{\partial z} = D \left( \frac{\partial^2 N}{\partial x^2} + \frac{\partial^2 N}{\partial y^2} + \frac{\partial^2 N}{\partial z^2} \right) + \sum_{n=1}^{N_{e,t}} R_n \quad (3.32)$$

#### 3.3.1 Time and grid volume averaging

The spatial domain in a model is divided into grid cells of finite size. Time is also divided into time steps of finite size for advancing species concentrations, velocities, and other variables. Real atmospheric motions generally occur over spatial scales much smaller than the resolution of model grid cells and over temporal scales smaller than the resolution of model time steps. For example, a typical mesoscale model might have horizontal resolution  $5 \text{ km} \times 5 \text{ km}$ , vertical resolution  $50 \text{ m}$ , and time resolution  $5 \text{ s}$ . A global-scale model might have horizontal resolution  $400 \text{ km} \times 400 \text{ km}$ , vertical resolution  $200 \text{ m}$ , and time resolution  $300 \text{ s}$ . Fluctuations in atmospheric motions due to eddies occur on smaller scales in both cases. Eddies (Section 4.2.6; Section 8.4), for example, range in diameter from a couple of millimeters to hundreds of meters and on time scales of seconds to hours.

Whereas many models do not resolve eddies, some do. These are discussed in Section 8.4. To account for subgrid-scale disturbances in those models that do not resolve eddies, a process called Reynolds averaging, named after Osborne Reynolds, is used. Models that treat turbulence using Reynolds averaging are called **Reynolds-averaged models**.



### 3.3 Expanded continuity equations

During Reynolds averaging, each variable in (3.32) and in other model equations is divided into an average and perturbation component. Such a division is referred to as **Reynolds decomposition**. In the case of gases, gas number concentration is decomposed as

$$N = \bar{N} + N' \quad (3.33)$$

where  $N$  is the **actual (precise or instantaneous) concentration**,  $\bar{N}$  is the **average concentration**, and  $N'$  is the **instantaneous perturbation concentration**. A precise concentration occurs at a given instant and location within a grid cell. An average concentration is obtained by integrating and averaging over a model time step and grid-cell volume. Thus,

$$\bar{N} = \frac{1}{h\Delta x\Delta y\Delta z} \int_t^{t+h} \left\{ \int_x^{x+\Delta x} \left[ \int_y^{y+\Delta y} \left( \int_z^{z+\Delta z} N \, dz \right) dy \right] dx \right\} dt \quad (3.34)$$

(e.g., Pielke 1984), where  $h$  is the time step, and  $\Delta x$ ,  $\Delta y$ ,  $\Delta z$  are space increments, shown in Fig. 3.2. The average concentrations are averages over one grid cell and time step and differ for each grid cell and time step. Perturbation concentrations are distributed on both sides of the average, so that the spatial and temporal average of all perturbations is zero ( $\bar{N}' = 0$ ), which is the **Reynolds assumption**.

Scalar and vector velocities can be decomposed in a similar manner. Thus, for example,

$$u = \bar{u} + u' \quad v = \bar{v} + v' \quad w = \bar{w} + w' \quad (3.35)$$

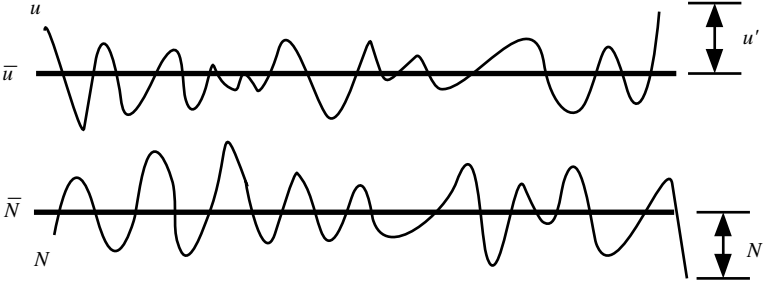
where  $\bar{u}$ ,  $\bar{v}$ , and  $\bar{w}$  are the time- and volume-averaged scalar velocities, and  $u'$ ,  $v'$ , and  $w'$  are perturbation scalar velocities, and

$$\bar{\mathbf{v}} = \bar{\mathbf{v}} + \mathbf{v}' \quad (3.36)$$

where  $\bar{\mathbf{v}} = \bar{u}\mathbf{i} + \bar{v}\mathbf{j} + \bar{w}\mathbf{k}$  is a time- and volume-averaged velocity and  $\mathbf{v}' = u'\mathbf{i} + v'\mathbf{j} + w'\mathbf{k}$  is a perturbation velocity. **Advection** is the mean horizontal velocity. Thus,  $\bar{u}$  and  $\bar{v}$  are components of advection. Figure 3.3 shows an example of precise, mean, and perturbation scalar velocities and trace-gas concentrations.

**Unsteady flow** occurs when  $\mathbf{v}$  varies with time, but not necessarily randomly, at a given location. **Steady flow** occurs when  $\mathbf{v}$  is independent of time. **Turbulent flow** is unpredictable flow in which  $\mathbf{v}$  varies randomly with time at a location. Thus, turbulent flow is unsteady, but unsteady flow is not necessarily turbulent. **Laminar flow** is nonturbulent flow in which  $\mathbf{v}$  may vary, but not randomly, with time at a given location. In laminar flow, fluid particles travel along well-defined streamlines and fluid layers flow independent of each other. Laminar flow can be steady or unsteady. Nearly all flows in the atmosphere are turbulent.

Subgrid-scale effects are estimated by substituting decomposed variables into an equation, then taking a time average and grid volume average of resulting terms. Substituting (3.33) and (3.35) into the species continuity equation from (3.32) and



**Figure 3.3** Precise, mean, and perturbation components of scalar velocity and gas concentration. The precise scalar velocity is denoted by  $u$ , the precise gas concentration is denoted by  $N$ , time- and volume-averaged values are denoted by an overbar, and perturbation components are denoted by a prime. Each point on the horizontal axis is a perturbation at a given time and location within a grid cell.

averaging terms over space and time (**Reynolds averaging**) give

$$\begin{aligned} & \left[ \frac{\partial(\bar{N} + N')}{\partial t} \right] + \left[ \frac{\partial(\bar{u} + u')(\bar{N} + N')}{\partial x} \right] + \left[ \frac{\partial(\bar{v} + v')(\bar{N} + N')}{\partial y} \right] \\ & + \left[ \frac{\partial(\bar{w} + w')(\bar{N} + N')}{\partial z} \right] = D \left\{ \left[ \frac{\partial^2(\bar{N} + N')}{\partial x^2} \right] + \left[ \frac{\partial^2(\bar{N} + N')}{\partial y^2} \right] \right. \\ & \left. + \left[ \frac{\partial^2(\bar{N} + N')}{\partial z^2} \right] \right\} + \sum_{n=1}^{N_{e,t}} R_n \end{aligned} \quad (3.37)$$

Since  $\overline{\partial(\bar{N} + N')/\partial t} = \partial(\bar{N} + N')/\partial t$ ,  $\overline{\bar{N} + N'} = \bar{N} + \bar{N}'$ ,  $\bar{N} = \bar{N}$ , and  $\bar{N}' = 0$ , the first term in (3.37) simplifies to

$$\left[ \frac{\partial(\bar{N} + N')}{\partial t} \right] = \frac{\partial(\bar{N} + \bar{N}')}{\partial t} = \frac{\partial \bar{N}}{\partial t} \quad (3.38)$$

Since  $\overline{u' \bar{N}} = 0$ ,  $\overline{\bar{u} N'} = 0$ , and  $\overline{\bar{u} \bar{N}} = \bar{u} \bar{N}$ , the second term simplifies to

$$\left[ \frac{\partial(\bar{u} + u')(\bar{N} + N')}{\partial x} \right] = \frac{\partial(\bar{u} \bar{N} + \bar{u} N' + u' \bar{N} + u' N')}{\partial x} = \frac{\partial(\bar{u} \bar{N} + u' N')}{\partial x} \quad (3.39)$$

The product  $\overline{u' N'}$  (m molec. cm<sup>-3</sup> s<sup>-1</sup>) represents the west–east transport of  $N'$  due to subgrid-scale eddies. It is a **kinematic turbulent flux** in that its units are those of concentration flux (kg [molec. cm<sup>-3</sup>] m<sup>-2</sup> s<sup>-1</sup>) divided by air density (kg m<sup>-3</sup>). When a variable or a flux is divided by the air density, it becomes a **kinematic variable** or flux. The partial derivative  $\partial(\overline{u' N'})/\partial x$  (molec. cm<sup>-3</sup> s<sup>-1</sup>) is a **turbulent flux divergence term**.

### 3.3 Expanded continuity equations

#### Example 3.2

Suppose two gas concentrations ( $N_1 = 8$  and  $N_2 = 4$ ) and scalar velocities ( $u_1 = 3$  and  $u_2 = -1$ ) are measured at different locations within a grid cell at a given time. Estimate  $\bar{N}$ ,  $N'_1$ ,  $N'_2$ ,  $\bar{u}$ ,  $u'_1$ ,  $u'_2$ ,  $\overline{u'N'}$ ,  $\bar{u}\bar{N}$ , and  $\overline{u\bar{N}}$ . Ignore units.

SOLUTION

$$\begin{aligned}\bar{N} &= (N_1 + N_2)/2 = 6 & \bar{u} &= (u_1 + u_2)/2 = 1 \\ N'_1 &= N_1 - \bar{N} = 2 & u'_1 &= u_1 - \bar{u} = 2 \\ N'_2 &= N_2 - \bar{N} = -2 & u'_2 &= u_2 - \bar{u} = -2 \\ \overline{u'N'} &= (u'_1 N'_1 + u'_2 N'_2)/2 = 4\bar{u}\bar{N} = 6 \\ \overline{u\bar{N}} &= \bar{u}\bar{N} + \overline{u'N'} = (u_1 N_1 + u_2 N_2)/2 = 10\end{aligned}$$

Substituting (3.38), (3.39), and similar terms for other directions into (3.37) gives

$$\begin{aligned}\frac{\partial \bar{N}}{\partial t} + \frac{\partial(\bar{u}\bar{N})}{\partial x} + \frac{\partial(\bar{v}\bar{N})}{\partial y} + \frac{\partial(\bar{w}\bar{N})}{\partial z} + \frac{\partial\overline{u'N'}}{\partial x} + \frac{\partial\overline{v'N'}}{\partial y} + \frac{\partial\overline{w'N'}}{\partial z} \\ = D \left( \frac{\partial^2 \bar{N}}{\partial x^2} + \frac{\partial^2 \bar{N}}{\partial y^2} + \frac{\partial^2 \bar{N}}{\partial z^2} \right) + \sum_{n=1}^{N_{e,t}} \bar{R}_n\end{aligned}\quad (3.40)$$

For motions larger than the molecular scale, the molecular diffusion terms in (3.40) are much smaller than are the turbulent flux divergence terms and can be removed. Thus, (3.40) simplifies to

$$\frac{\partial \bar{N}}{\partial t} + \frac{\partial(\bar{u}\bar{N})}{\partial x} + \frac{\partial(\bar{v}\bar{N})}{\partial y} + \frac{\partial(\bar{w}\bar{N})}{\partial z} + \frac{\partial\overline{u'N'}}{\partial x} + \frac{\partial\overline{v'N'}}{\partial y} + \frac{\partial\overline{w'N'}}{\partial z} = \sum_{n=1}^{N_{e,t}} \bar{R}_n \quad (3.41)$$

which compresses to the **continuity equation for a gas**,

$$\frac{\partial \bar{N}}{\partial t} + \nabla \cdot (\bar{\mathbf{v}}\bar{N}) + \nabla \cdot (\overline{\mathbf{v}'N'}) = \sum_{n=1}^{N_{e,t}} \bar{R}_n \quad (3.42)$$

An analogous equation for air density results in the **continuity equation for air**,

$$\frac{\partial \bar{\rho}_a}{\partial t} + \nabla \cdot (\bar{\mathbf{v}}\bar{\rho}_a) + \nabla \cdot (\overline{\mathbf{v}'\rho'_a}) = 0 \quad (3.43)$$

In (3.43), the external source and sink terms for air molecules are neglected because they are small in comparison with the other terms.

Equation (3.42) can be rederived in terms of moist-air mass mixing ratio. Adding source and sink terms to (3.26) yields

$$\frac{\partial q}{\partial t} + \mathbf{v} \cdot \nabla q = \sum_{n=1}^{N_{e,t}} R_n \quad (3.44)$$

where  $R_n$  is now in kilograms per kilogram of moist air per second. Multiplying the continuity equation for air from (3.20) by  $q$ , multiplying (3.44) by  $\rho_a$ , adding the results, and compressing give

$$\frac{\partial(\rho_a q)}{\partial t} + \nabla \cdot (\rho_a \mathbf{v} q) = \rho_a \sum_{n=1}^{N_{e,t}} R_n \quad (3.45)$$

The moist-air mass mixing ratio, velocity, and density can be decomposed with  $q = \bar{q} + q'$ ,  $\mathbf{v} = \bar{\mathbf{v}} + \mathbf{v}'$ , and  $\rho_a = \bar{\rho}_a + \rho'_a$ , respectively. Density perturbations in the atmosphere are relatively small; thus,  $\rho'_a \ll \bar{\rho}_a$ , and  $\rho_a \approx \bar{\rho}_a$ . Substituting decomposed variable values into all but the  $R$  term in (3.45) gives

$$\frac{\partial[\bar{\rho}_a(\bar{q} + q')]}{\partial t} + \nabla \cdot [\bar{\rho}_a(\bar{\mathbf{v}} + \mathbf{v}')(\bar{q} + q')] = \bar{\rho}_a \sum_{n=1}^{N_{e,t}} R_n \quad (3.46)$$

Taking the time and grid volume average of this equation, eliminating zero-value terms and removing unnecessary overbars results in

$$\bar{\rho}_a \left[ \frac{\partial \bar{q}}{\partial t} + (\bar{\mathbf{v}} \cdot \nabla) \bar{q} \right] + \bar{q} \left[ \frac{\partial \bar{\rho}_a}{\partial t} + \nabla \cdot (\bar{\mathbf{v}} \bar{\rho}_a) \right] + \nabla \cdot (\bar{\rho}_a \overline{\mathbf{v}' q'}) = \bar{\rho}_a \sum_{n=1}^{N_{e,t}} \bar{R}_n \quad (3.47)$$

Equation (3.47) can be simplified by first noting that, when  $\rho'_a \ll \bar{\rho}_a$ , (3.43) becomes

$$\frac{\partial \bar{\rho}_a}{\partial t} + \nabla \cdot (\bar{\mathbf{v}} \bar{\rho}_a) = 0 \quad (3.48)$$

Substituting this expression into (3.47) and dividing through by  $\bar{\rho}_a$  give

$$\frac{\partial \bar{q}}{\partial t} + (\bar{\mathbf{v}} \cdot \nabla) \bar{q} + \frac{1}{\bar{\rho}_a} \nabla \cdot (\bar{\rho}_a \overline{\mathbf{v}' q'}) = \sum_{n=1}^{N_{e,t}} \bar{R}_n \quad (3.49)$$

which is the **gas continuity equation** in units of the moist-air mass mixing ratio.

In (3.49),  $\overline{u'q'}$ ,  $\overline{v'q'}$ , and  $\overline{w'q'}$  (m kg kg<sup>-1</sup> s<sup>-1</sup>) are **kinematic turbulent fluxes** of mixing ratio. Whereas models calculate spatially and temporally averaged values (e.g.,  $\bar{N}$ ,  $\bar{q}$ ,  $\bar{\rho}_a$ ,  $\bar{u}$ ), kinematic turbulent fluxes (e.g.,  $\overline{u'N'}$ ) are parameterized. Some parameterizations are discussed in Section 8.4. Here, a simple overview of  $K$ -theory is given.

With  **$K$ -theory** (gradient transport theory), kinematic turbulent fluxes are replaced with the product of a constant and the gradient of the mean value of a fluctuating variable (Calder 1949; Pasquill 1962; Monin and Yaglom 1971; Reynolds *et al.* 1973; Stull 1988). This is convenient, because models predict mean quantities.

### 3.3 Expanded continuity equations

Kinematic turbulent fluxes of gas concentration, for example, are parameterized with

$$\overline{w'N'} = -K_{b,xx} \frac{\partial \bar{N}}{\partial x} \quad \overline{v'N'} = -K_{b,yy} \frac{\partial \bar{N}}{\partial y} \quad \overline{w'N'} = -K_{b,zz} \frac{\partial \bar{N}}{\partial z} \quad (3.50)$$

where  $K_{b,xx}$ ,  $K_{b,yy}$ , and  $K_{b,zz}$  (e.g.,  $\text{cm}^2 \text{s}^{-1}$ ) are **eddy diffusion coefficients** in the  $x$ -,  $y$ -, and  $z$ -directions, respectively. The subscript  $b$  indicates that the **eddy diffusion coefficient for energy** (eddy thermal diffusivity) is used. The eddy diffusion coefficient for energy is used because the turbulent transport of a gas is similar to that of energy. When turbulent transport of velocity is simulated, an **eddy diffusion coefficient for momentum** (eddy viscosity) term is used. Eddy diffusion coefficients for energy and momentum differ, but not by much. Eddy diffusion coefficients represent an average diffusion coefficient for eddies of all sizes smaller than the grid cell. Eddy diffusion coefficients are also called eddy transfer, eddy exchange, turbulent transfer, and gradient transfer coefficients.

Eddy diffusion coefficients are parameterizations of subgrid scale transport of energy and momentum. In the vertical, such transport is caused by **mechanical shear** (mechanical turbulence) and/or **buoyancy** (thermal turbulence). Horizontal wind shear creates eddies that increase in size when the wind flows over rough surfaces. Buoyancy creates instability, causing shear-induced eddies to become wider and taller. Vertical motions in eddies transfer surface air upward and air aloft downward. Eddies also exchange air horizontally.

Substituting (3.50) into (3.41) gives

$$\begin{aligned} \frac{\partial \bar{N}}{\partial t} + \frac{\partial(\bar{u}\bar{N})}{\partial x} + \frac{\partial(\bar{v}\bar{N})}{\partial y} + \frac{\partial(\bar{w}\bar{N})}{\partial z} \\ = \frac{\partial}{\partial x} \left( K_{b,xx} \frac{\partial \bar{N}}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{b,yy} \frac{\partial \bar{N}}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_{b,zz} \frac{\partial \bar{N}}{\partial z} \right) + \sum_{n=1}^{N_{e,t}} \bar{R}_n \end{aligned} \quad (3.51)$$

Compressing (3.51) and removing overbars for simplicity give the **continuity equation for an individual gas in number concentration units** and Cartesian-altitude coordinates as

$$\frac{\partial N}{\partial t} + \nabla \cdot (\mathbf{v}N) = (\nabla \cdot \mathbf{K}_b \nabla) N + \sum_{n=1}^{N_{e,t}} R_n \quad (3.52)$$

where

$$\mathbf{K}_b = \begin{bmatrix} K_{b,xx} & 0 & 0 \\ 0 & K_{b,yy} & 0 \\ 0 & 0 & K_{b,zz} \end{bmatrix} \quad (3.53)$$

is the eddy diffusion tensor for energy. The analogous continuity equation for an individual gas in moist-air mass mixing ratio units is

$$\frac{\partial q}{\partial t} + (\mathbf{v} \cdot \nabla)q = \frac{1}{\rho_a}(\nabla \cdot \rho_a \mathbf{K}_b \nabla)q + \sum_{n=1}^{N_{e,t}} R_n \quad (3.54)$$

The units of  $R_n$  differ in the two cases.

### 3.3.2 Continuity equation for air

External sources and sinks ( $R_n$ ) are relatively small and can be ignored in the continuity equation for air. For most modeling applications, the turbulent flux divergence term in the equation can also be ignored because  $\rho'_a \ll \bar{\rho}_a$ . After removing overbars for convenience and making the above modifications, the continuity equation for air in Cartesian-altitude coordinates reduces from (3.43) to

$$\frac{\partial \rho_a}{\partial t} + \nabla \cdot (\mathbf{v} \rho_a) = 0 \quad (3.55)$$

### 3.3.3 Gas continuity equation

The continuity equations for trace gases and particles include several external source and sink terms. Gases enter the atmosphere from surface and elevated sources by **emission**. They are removed onto water, soil, foliage, roads, buildings, cars, and other surfaces by **dry deposition**. In many cases, gases are swept out of the atmosphere by falling raindrops during **washout**. Gases react chemically with each other and are dissociated by solar radiation during **photochemistry**. Some gases aggregate to form new particles during **homogeneous nucleation** or aggregate on existing particle surfaces during **heterogeneous nucleation**. Once a surface has nucleated, gas molecules may diffuse to and **condense** as a liquid or **deposit** as a solid on the surface. Liquid material may also **evaporate** or solid material may **sublimate** to the gas phase. A gas may also **dissolve** in liquid water on the surface of a particle. Dissolved gases may evaporate. Finally, a gas may react chemically on the surface of a particle during **heterogeneous chemistry**.

A form of the continuity equation for a gas  $q$  that accounts for the processes discussed above is

$$\begin{aligned} \frac{\partial N_q}{\partial t} + \nabla \cdot (\mathbf{v} N_q) = & (\nabla \cdot \mathbf{K}_b \nabla) N_q \\ & + R_{\text{emisg}} + R_{\text{depg}} + R_{\text{washg}} + R_{\text{chemg}} \\ & + R_{\text{nucg}} + R_{\text{c/eg}} + R_{\text{dp/sg}} + R_{\text{ds/eg}} + R_{\text{hrg}} \end{aligned} \quad (3.56)$$

### 3.3 Expanded continuity equations

where

$R_{\text{emisg}}$  = rate of surface or elevated emission

$R_{\text{depg}}$  = rate of dry deposition to the ground

$R_{\text{washg}}$  = rate of washout to the ground or from one altitude to another

$R_{\text{chemg}}$  = rate of photochemical production or loss

$R_{\text{nucg}}$  = rate of gas loss due to homogeneous or heterogeneous nucleation

$R_{\text{c/eg}}$  = rate of gas loss (production) due to condensation (evaporation)

$R_{\text{dp/sg}}$  = rate of gas loss (production) due to depositional growth (sublimation)

$R_{\text{ds/eg}}$  = rate of gas loss (production) due to dissolutational growth (evaporation)

$R_{\text{hrg}}$  = rate of gas loss (production) due to heterogeneous reactions

All rates are expressed in units of concentration per unit time (e.g., molec.  $\text{cm}^{-3} \text{s}^{-1}$ ).

#### 3.3.4 Particle continuity equation

The continuity equation for particles is divided into two subequations. One is for particle number concentration, and the other is for particle volume component concentration. Particles contain anywhere from one to hundreds of components. The volume of each component varies over time due to physical and chemical processes. If the total volume of one particle in a size bin  $i$  is denoted by  $v_i$  ( $\text{cm}^3/\text{particle}$ ), the **volume** of component  $q$  within that particle is  $v_{q,i}$ . Thus,  $v_{q,i}$  gives information about a component in a single particle of a given size. A variable giving information about that component summed over all particles of the same size, is more relevant. Such a parameter is **volume concentration** (cubic centimeters of the component per cubic centimeter of air), defined as

$$v_{q,i} = n_i v_{q,i} \quad (3.57)$$

where  $n_i$  is the **number concentration** of particles of size  $i$  (particles per cubic centimeter of air). If two of the three variables in (3.57) are predicted numerically, the third can be found from the equation. Typically, volume concentration and number concentration are predicted numerically. They are found from separate continuity equations, because different external sources and sinks affect the number and volume concentrations.

The continuity equation for the number concentration of particles of size  $i$  is

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (v n_i) = (\nabla \cdot \mathbf{K}_b \nabla) n_i + R_{\text{emisg}} + R_{\text{depg}} + R_{\text{sedn}} + R_{\text{washg}} + R_{\text{nucg}} + R_{\text{coagn}} \quad (3.58)$$

where

$R_{\text{emisn}}$  = rate of surface or elevated emission

$R_{\text{depn}}$  = rate of particle dry deposition to the surface

$R_{\text{sedn}}$  = rate of sedimentation to the surface or between layers

$R_{\text{washn}}$  = rate of washout to the surface or from one altitude down to another

$R_{\text{nucn}}$  = rate of production of new particles due to homogeneous nucleation

$R_{\text{coagn}}$  = rate of coagulation of number concentration

All rates are in units of particles  $\text{cm}^{-3} \text{ s}^{-1}$ . Sources and sinks that affect particle number concentration include emission, dry deposition, sedimentation, washout, homogeneous nucleation, and coagulation. **Sedimentation** occurs when particles fall through the atmosphere due to their mass. Sedimentation by gases is negligible because gas molecules have extremely small masses. **Particle dry deposition** occurs when particles diffuse to or otherwise impact a surface by any transport process. **Particle washout** occurs when rain sweeps particles in its path to lower altitudes or the surface. **Homogeneous nucleation** is a source of new particles. **Heterogeneous nucleation** does not produce new particles but allows growth to proceed on existing particles. **Coagulation** occurs when two particles collide and stick to form a single, larger particle.

The continuity equation for the volume concentration of component  $q$  in particles of size  $i$  is

$$\frac{\partial v_{q,i}}{\partial t} + \nabla \cdot (\mathbf{v}v_{q,i}) = (\nabla \cdot \mathbf{K}_b \nabla) v_{q,i} + R_{\text{emisv}} + R_{\text{depv}} + R_{\text{sedv}} + R_{\text{washv}} + R_{\text{nucv}} + R_{\text{coagv}} + R_{\text{c/ev}} + R_{\text{dp/sv}} + R_{\text{ds/ev}} + R_{\text{eqv}} + R_{\text{aqv}} + R_{\text{hrv}} \quad (3.59)$$

where

$R_{\text{emisv}}$  = rate of surface or elevated emission

$R_{\text{depv}}$  = rate of dry deposition to the surface

$R_{\text{sedv}}$  = rate of sedimentation to the surface or from one altitude to another

$R_{\text{washv}}$  = rate of washout to the surface or from one altitude to another

$R_{\text{nucv}}$  = rate of change due to homogeneous or heterogeneous nucleation

$R_{\text{coagv}}$  = rate of change due to coagulation

$R_{\text{c/ev}}$  = rate of change due to condensational growth (evaporation)

$R_{\text{dp/sv}}$  = rate of change due to depositional growth (sublimation)

$R_{\text{ds/ev}}$  = rate of change due to dissolutional growth (evaporation)

$R_{\text{eqv}}$  = rate of change due to reversible chemical equilibrium reactions

$R_{\text{aqv}}$  = rate of change due to irreversible aqueous chemical reactions

$R_{\text{hrv}}$  = rate of change due to heterogeneous reactions on particle surfaces

Rates in this equation have units of cubic centimeters of component  $q$  per cubic centimeter of air per second. Some processes, such as homogeneous nucleation and coagulation, affect number and volume concentrations. Others, such as



### 3.3 Expanded continuity equations

heterogeneous nucleation, condensation, deposition, dissolution, heterogeneous reaction, chemical equilibrium and aqueous chemistry affect volume concentration but not number concentration.

#### 3.3.5 Continuity equation for gas, liquid, and solid water

Water in the atmosphere appears as a gas, liquid, or solid. In a model, the total water content is estimated as

$$q_T = q_v + \sum_{i=1}^{N_B} (q_{L,i} + q_{I,i}) \quad (3.60)$$

where  $N_B$  is the number of particle size categories (bins),  $q_v$  is the specific humidity of water vapor (kilograms per kilogram of moist air),  $q_{L,i}$  is the moist-air mass mixing ratio of liquid water in a size bin, and  $q_{I,i}$  is the moist-air mass mixing ratio of ice in a size bin. Mass mixing ratios are determined from the continuity equations for water vapor, liquid, and ice,

$$\begin{aligned} \frac{\partial q_v}{\partial t} + (\mathbf{v} \cdot \nabla) q_v &= \frac{1}{\rho_a} (\nabla \rho_a \mathbf{K}_b \nabla) q_v \\ &+ R_{emisV} + R_{depV} + R_{chemV} + R_{c/eV} + R_{dp/sV} \end{aligned} \quad (3.61)$$

$$\begin{aligned} \frac{\partial q_{L,i}}{\partial t} + (\mathbf{v} \cdot \nabla) q_{L,i} &= \frac{1}{\rho_a} (\nabla \rho_a \mathbf{K}_b \nabla) q_{L,i} + R_{emisL} + R_{depL} \\ &+ R_{sedL} + R_{coagL} + R_{c/eL} + R_{f/mL} \end{aligned} \quad (3.62)$$

$$\begin{aligned} \frac{\partial q_{I,i}}{\partial t} + (\mathbf{v} \cdot \nabla) q_{I,i} &= \frac{1}{\rho_a} (\nabla \rho_a \mathbf{K}_b \nabla) q_{I,i} \\ &+ R_{depI} + R_{sedI} + R_{coagI} + R_{f/ml} + R_{dp/sl} \end{aligned} \quad (3.63)$$

where

$R_{emis}$  = rate of surface or elevated emission

$R_{dep}$  = rate of dry deposition to the surface

$R_{sed}$  = rate of sedimentation to the surface or from one altitude to another

$R_{chem}$  = rate of photochemical production or loss

$R_{coag}$  = rate of liquid or ice production or loss in a size bin due to coagulation

$R_{c/e}$  = rate of change due to condensational growth (evaporation)

$R_{dp/s}$  = rate of change due to depositional growth (sublimation)

$R_{f/m}$  = rate of change due to freezing (melting)

and the units of  $R$  are kilograms per kilogram of moist air per second.

Many meteorological models simulate liquid water and ice as **bulk parameters**. In such cases, liquid water and ice are not separated into size categories, and their number concentrations are not tracked. Instead, only the moist-air mass mixing ratios of total liquid water and ice are predicted. Since particles are not size-resolved in a bulk parameterization, some processes, such as coagulation, cannot be treated adequately. When liquid and ice content are treated as bulk parameters,

$q_T = q_v + q_L + q_I$ , where the subscript  $i$  has been dropped because a bulk parameterization has no size resolution.

### 3.4 THERMODYNAMIC ENERGY EQUATION

Air **temperature** is affected by energy transfer and work. Energy transfer processes include conduction, mechanical turbulence, thermal turbulence, advection, and radiation, all introduced in Section 2.2. Energy is released to the air during condensation of water vapor, deposition of water vapor, freezing of liquid water, exothermic chemical reactions, and radioactive decay. Energy is removed from the air upon melting of ice, sublimation of ice, and evaporation of liquid water. Energy exchange may also occur upon the change of state of substances other than water. Because the quantities of nonwater substances changing state are relatively small, resulting energy exchanges are small. Energy, like air density and species concentrations, is conserved in a system.

An equation describing energy changes in the atmosphere can be derived by combining the first law of thermodynamics with the continuity equation for air. The first law of thermodynamics as expressed in (2.82) was  $dQ \approx c_{p,d} dT_v - \alpha_a dp_a$ . Differentiating this equation with respect to time, substituting  $\alpha_a = 1/\rho_a$ , and rearranging give the **thermodynamic energy equation** as

$$\frac{dT_v}{dt} \approx \frac{1}{c_{p,d}} \frac{dQ}{dt} + \frac{1}{c_{p,d}\rho_a} \frac{dp_a}{dt} \quad (3.64)$$

If the thermodynamic energy equation is written in terms of potential virtual temperature, the last term in (3.64) can be eliminated. Differentiating  $\theta_v = T_v(1000/p_a)^\kappa$  with respect to time give

$$\frac{d\theta_v}{dt} = \frac{dT_v}{dt} \left( \frac{1000}{p_a} \right)^\kappa + T_v \kappa \left( \frac{1000}{p_a} \right)^{\kappa-1} \left( -\frac{1000}{p_a^2} \right) \frac{dp_a}{dt} = \frac{\theta_v}{T_v} \frac{dT_v}{dt} - \frac{\kappa\theta_v}{p_a} \frac{dp_a}{dt} \quad (3.65)$$

Substituting (3.65),  $\kappa = R'/c_{p,d}$ , and  $p_a = \rho_a R' T_v$  into (3.64), and expanding the total derivative with (3.13) give the thermodynamic energy equation in terms of potential virtual temperature as

$$\frac{d\theta_v}{dt} = \frac{\partial\theta_v}{\partial t} + (\mathbf{v} \cdot \nabla)\theta_v \approx \frac{\theta_v}{c_{p,d}T_v} \frac{dQ}{dt} \quad (3.66)$$

Multiplying all terms in (3.66) by  $c_{p,d}\rho_a$ , multiplying all terms in the continuity equation for air from (3.20) by  $c_{p,d}\theta_v$ , adding the two equations, and compressing give

$$\frac{\partial(c_{p,d}\rho_a\theta_v)}{\partial t} + \nabla \cdot (\mathbf{v}c_{p,d}\rho_a\theta_v) \approx \rho_a \frac{\theta_v}{T_v} \frac{dQ}{dt} \quad (3.67)$$

### 3.4 Thermodynamic energy equation

Substituting the **energy density** ( $\text{J m}^{-3}$ ), defined as  $E = c_{p,d}\rho_a\theta_v$ , into (3.67) gives the **continuity equation for energy**,

$$\frac{\partial E}{\partial t} + \nabla \cdot (\mathbf{v}E) \approx \rho_a \frac{\theta_v}{T_v} \frac{dQ}{dt} \quad (3.68)$$

This equation is similar to the continuity equations for air mass density or gas number concentration. It states that the time rate of change of energy in a box equals the energy flux in minus the energy flux out plus (minus) external sources (sinks). Replacing  $N$  with  $E$  in Fig. 3.2 yields a diagram of energy fluxes into and out of a hypothetical grid cell.

In a model, subgrid eddies affect energy transport. To account for such eddies, variables in (3.67) can be decomposed as  $\mathbf{v} = \bar{\mathbf{v}} + \mathbf{v}'$ ,  $\rho_a = \bar{\rho}_a + \rho'_a$  and  $\theta_v = \bar{\theta}_v + \theta'_v$ . Since density perturbations are small ( $\rho'_a \ll \bar{\rho}_a$ ), density is approximated as  $\rho_a \approx \bar{\rho}_a$ . Substituting velocity, density, and potential virtual temperature decompositions into (3.67), setting the approximation to an equal sign for simplicity, and taking the time- and grid-volume average of the result yield

$$c_{p,d} \left\{ \overline{\frac{\partial[\bar{\rho}_a(\bar{\theta}_v + \theta'_v)]}{\partial t}} \right\} + c_{p,d} \overline{\nabla \cdot [\bar{\rho}_a(\bar{\mathbf{v}}\bar{\theta}_v + \bar{\mathbf{v}}\theta'_v + \mathbf{v}'\bar{\theta}_v + \mathbf{v}'\theta'_v)]} = \bar{\rho}_a \frac{\theta_v}{T_v} \frac{dQ}{dt} \quad (3.69)$$

Eliminating zero-value time and spatial derivatives and unnecessary overbars results in

$$\frac{\partial(\bar{\rho}_a\bar{\theta}_v)}{\partial t} + \nabla \cdot (\bar{\rho}_a\bar{\mathbf{v}}\bar{\theta}_v) + \overline{\nabla \cdot (\bar{\rho}_a\mathbf{v}'\theta'_v)} = \frac{\bar{\rho}_a}{c_{p,d}} \frac{\theta_v}{T_v} \frac{dQ}{dt} \quad (3.70)$$

which expands to

$$\bar{\rho}_a \left[ \frac{\partial\bar{\theta}_v}{\partial t} + (\bar{\mathbf{v}} \cdot \nabla) \bar{\theta}_v \right] + \bar{\theta}_v \left[ \frac{\partial\bar{\rho}_a}{\partial t} + \nabla \cdot (\bar{\mathbf{v}}\bar{\rho}_a) \right] + \nabla \cdot (\bar{\rho}_a\mathbf{v}'\theta'_v) = \frac{\bar{\rho}_a}{c_{p,d}} \frac{\theta_v}{T_v} \frac{dQ}{dt} \quad (3.71)$$

Substituting the continuity equation for air from (3.48) into (3.71) and dividing by  $\bar{\rho}_a$  give the thermodynamic energy equation as

$$\frac{\partial\bar{\theta}_v}{\partial t} + (\bar{\mathbf{v}} \cdot \nabla) \bar{\theta}_v + \frac{1}{\bar{\rho}_a} \nabla \cdot (\bar{\rho}_a\mathbf{v}'\theta'_v) = \frac{\theta_v}{c_{p,d}T_v} \frac{dQ}{dt} \quad (3.72)$$

The kinematic turbulent sensible-heat fluxes ( $\overline{\mathbf{v}'\theta'_v}$ ) can be parameterized with

$$\overline{u'\theta'_v} = -K_{b,xx} \frac{\partial\bar{\theta}_v}{\partial x} \quad \overline{v'\theta'_v} = -K_{b,yy} \frac{\partial\bar{\theta}_v}{\partial y} \quad \overline{w'\theta'_v} = -K_{b,zz} \frac{\partial\bar{\theta}_v}{\partial z} \quad (3.73)$$

where the eddy diffusion coefficients for energy are the same as those used in the continuity equation for a trace species. Substituting  $\overline{\mathbf{v}'\theta'_v} = -\mathbf{K}_b \nabla \bar{\theta}_v$  into (3.72) and eliminating overbars for simplicity give

$$\frac{\partial\theta_v}{\partial t} + (\mathbf{v} \cdot \nabla)\theta_v = \frac{1}{\rho_a} (\nabla \cdot \rho_a \mathbf{K}_b \nabla)\theta_v + \frac{\theta_v}{c_{p,d}T_v} \frac{dQ}{dt} \quad (3.74)$$

The diabatic heating rate consists of the terms

$$\frac{dQ}{dt} = \sum_{n=1}^{N_{e,h}} \frac{dQ_n}{dt} = \frac{dQ_{c/e}}{dt} + \frac{dQ_{f/m}}{dt} + \frac{dQ_{dp/s}}{dt} + \frac{dQ_{\text{solar}}}{dt} + \frac{dQ_{\text{ir}}}{dt} \quad (3.75)$$

where  $N_{e,h}$  is the number of diabatic energy sources and sinks. All  $Q$ 's are in joules per kilogram.  $dQ_{c/e}/dt$  is the rate of energy release (absorption) due to condensation (evaporation),  $dQ_{f/m}/dt$  is the rate of energy release (absorption) due to freezing (melting),  $dQ_{dp/s}/dt$  is the rate of energy release (absorption) due to deposition (sublimation),  $dQ_{\text{solar}}/dt$  is the rate of solar heating, and  $dQ_{\text{ir}}/dt$  is the rate of net infrared heating (cooling). Substituting (3.75) into (3.74) gives the **thermodynamic energy equation** as

$$\frac{\partial \theta_v}{\partial t} + (\mathbf{v} \cdot \nabla) \theta_v = \frac{1}{\rho_a} (\nabla \cdot \rho_a \mathbf{K}_b \nabla) \theta_v + \frac{\theta_v}{c_{p,d} T_v} \sum_{n=1}^{N_{e,h}} \frac{dQ_n}{dt} \quad (3.76)$$

### 3.5 SUMMARY

In this chapter, local and total derivatives were defined, and the continuity and thermodynamic energy equations were derived. Continuity equations included those for air, trace gases, aerosol number concentration, and aerosol volume concentration. These equations treat subgrid eddy motions with kinematic turbulent flux terms, which are generally parameterized. A common type of parameterization is a  $K$ -theory parameterization. Equations described in this chapter are necessary for simulating the transport and transformations of total air, gases, aerosol particles, and energy. An equation used for predicting wind speed and direction, the momentum equation, is discussed next.

### 3.6 PROBLEMS

- 3.1** Expand the total derivative of the  $u$ -scalar velocity (i.e., substitute  $u$  for  $N$  in (3.5)) when the air flow is (a) steady, (b) unsteady.
- 3.2** Explain why (3.17) differs from (3.26).
- 3.3** What is the purpose of Reynolds averaging?
- 3.4** If  $u = -5 \text{ m s}^{-1}$  and  $v = +5 \text{ m s}^{-1}$ , write out the horizontal velocity vector, determine the horizontal wind speed, and name the wind.
- 3.5** Assume that a grid cell has dimension  $\Delta x = 5 \text{ km}$ ,  $\Delta y = 4 \text{ km}$ , and  $\Delta z = 0.1 \text{ km}$  and that the west, east, south, north, and lower scalar velocities are  $u_1 = +3$ ,  $u_2 = +4$ ,  $v_3 = -3$ ,  $v_4 = +2$ , and  $w_5 = +0.2 \text{ m s}^{-1}$ . If the atmosphere is incompressible, what is  $w$  at the top of the cell?
- 3.6 (a)** A grid cell has dimensions  $\Delta x = 5 \text{ km}$ ,  $\Delta y = 4 \text{ km}$ , and  $\Delta z = 0.1 \text{ km}$ . Assume the gas concentration and scalar velocity at the west boundary of the cell are  $N_1 = 1 \times 10^{11} \text{ molec. cm}^{-3}$  and  $u_1 = +7 \text{ m s}^{-1}$ , respectively, and those at the east boundary of the cell are  $N_2 = 5 \times 10^{11} \text{ molec. cm}^{-3}$  and  $u_2 = +8 \text{ m s}^{-1}$ , respectively. (i) Assuming external sources and sinks

### 3.7 Computer programming practice

and eddy diffusion are absent, estimate  $N$  at the cell center after 60 s if the initial  $N$  is an average of the two boundary  $N$ -values and boundary parameters remain constant. (ii) Calculate the time after the start at which  $N$  at the cell center becomes zero.

- (b) Assume that the gas concentration and scalar velocity at the south boundary of the grid cell in part (a) are  $N_3 = 1 \times 10^{11}$  molec.  $\text{cm}^{-3}$  and  $v_3 = -2$   $\text{m s}^{-1}$ , respectively, and those at the north boundary are  $N_4 = 7 \times 10^{11}$  molec.  $\text{cm}^{-3}$  and  $v_4 = +1$   $\text{m s}^{-1}$ , respectively. Calculate (i)  $N$  at the cell center after 60 s and (ii) the time after the start at which  $N$  at the center becomes zero. Assume fluxes operate in four directions, and the initial  $N$  at the center of the cell is the average of all four grid-boundary  $N$ -values.
- (c) Convert the gas number concentrations from part (a) ( $N_1$  and  $N_2$ ) to moist-air mass mixing ratios, assuming that the gas is ozone,  $T_v = 298$  K, and  $p_a = 1013$  hPa.
- (d) Re-solve parts (a) (i) and (a) (ii) with (3.26) using moist-air mass mixing ratios instead of number concentration units. Assume that the west–east velocity for this question is an average of the grid-cell boundary velocities. Convert the mass mixing ratio from the 60-s case back to number concentration units. How does the result compare with that found in part (a) (i)? If it differs, why does it differ?
- 3.7** A grid cell has dimensions  $\Delta x = 5$  km,  $\Delta y = 4$  km, and  $\Delta z = 0.1$  km. Assume that the potential virtual temperature, pressure, and scalar velocity at the west boundary of the grid cell are  $\theta_{v,1} = 302$  K,  $p_{a,1} = 1004$  hPa, and  $u_1 = +7$   $\text{m s}^{-1}$ , respectively, and those at the east boundary of the grid cell are  $\theta_{v,2} = 299$  K,  $p_{a,2} = 1008$  hPa, and  $u_2 = +8$   $\text{m s}^{-1}$ , respectively.
- (a) Calculate the virtual temperature and air density at the west and east boundaries of the grid cell.
- (b) Calculate the energy density  $E$  at each boundary.
- (c) Assuming diabatic energy sources and sinks and eddy diffusion are absent, calculate the potential virtual temperature at the center of the grid cell after 10 s.

### 3.7 COMPUTER PROGRAMMING PRACTICE

- 3.8** Assume that grid-cell size, boundary conditions, and  $N$  are initially the same as in Problem 3.6(a). Write a computer script to calculate the final  $N$  at the grid-cell center after a time step  $h$ . After each time step, set the east-boundary gas concentration ( $N_2$ ) equal to the final concentration at the center of the cell. Set  $h = 3$  s, and run the program for a simulation period of one hour. Plot the grid center concentration versus time.
- 3.9** Assume that grid-cell size, boundary conditions, and initial  $\theta_v$  are the same as in Problem 3.7. Write a computer script to calculate the final  $\theta_v$  at the cell center after a time step  $h$ . After each step, set  $\theta_{v,2}$  equal to  $\theta_v$  at the cell center. Set  $h = 3$  s, and run the program for six hours. Plot  $\theta_v$  versus time at the cell center.