Incorporating the Work Done by Vertical Density Fluxes in Both Kinetic and Thermal Energy Conservation Equations to Satisfy Total Energy Conservation

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ABSTRACT

Conservation of total, kinetic, and thermal energy in the atmosphere is revisited, and the derived thermal energy balance is examined with observations. Total energy conservation (TEC) provides a constraint for the sum of kinetic, thermal, and potential energy changes. In response to air thermal expansion/compression, air density variation leads to vertical density fluxes and potential energy changes, which in turn impact the thermal energy balance as well as the kinetic energy balance due to the constraint of TEC. As vertical density fluxes can propagate through a large vertical domain to where local thermal expansion/compression becomes negligibly small, interactions between kinetic and thermal energy changes in determining atmospheric motions and thermodynamic structures can occur when local diabatic heating/cooling becomes small. The contribution of vertical density fluxes to the kinetic energy balance is sometimes considered but that to the thermal energy balance is traditionally missed. Misinterpretation between air thermal expansion/compression and incompressibility for air volume changes with pressure under a constant temperature would lead to overlooking important impacts of thermal expansion/compression on air motions and atmospheric thermodynamics. Atmospheric boundary layer observations qualitatively confirm the contribution of potential energy changes associated with vertical density fluxes in the thermal energy balance for explaining temporal variations of air temperature.

1. Introduction

Interactions between thermal and kinetic energy changes have been historically investigated in the literature under available potential energy, for example, by Margules (1910) and Lorenz (1955). The focus of available potential energy is mainly on the hydrostatically balanced atmosphere so far. Zilitinkevich et al. (2007) proposed the idea of total turbulent energy conservation by considering interactions between turbulent kinetic energy (TKE) and turbulent potential energy (TPE) changes, in which TPE is defined as the temperature variance normalized by the Brunt–Väisälä frequency. Because turbulent mixing is a process that results from the nonhydrostatic pressure balance, essentially Zilitinkevich et al. (2007) have extended the investigation of interactions between kinetic and thermal energy changes to the nonhydrostatic atmosphere. Note that total turbulence energy (TTE) defined by Zilitinkevich et al. (2007) as the sum of TKE and TPE is different from total energy conservation, which is described in this study, and TTE is not constrained by an independent conservation law.

By analyzing observed turbulent mixing in the atmospheric boundary layer, Sun et al. (2016) found that interactions between atmospheric kinetic and thermal energy changes are crucial in determining turbulence intensity, and turbulent mixing plays an important role in heat transfer for temperature redistribution and the atmospheric stratification. In addition, they demonstrated that the most energetic turbulence eddies are large and nonlocal. Their study stresses the important role of energy conservation in determining air motion and atmospheric thermodynamic structures. However, using the traditional thermal energy conservation equation, we are unable to explain observed diurnal variations of air temperature even for a simple sunny day over a flat homogeneous terrain (see details in section 4). The unsatisfactory theoretical explanation of the observation leads us to examine thermal energy conservation for the atmosphere in this study.

In the literature, names of conservation laws have been used differently; we first clarify those names. Note that all the energy conservation laws address the balance

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between energy changes or the rate of energy, and environmental forcings, not energy itself, are conserved unless the net forcing is zero. Kinetic energy conservation describes the balance between the net change of kinetic energy or the rate of kinetic energy within a system of a finite volume and the net change of work done at the boundary of the system. Following classical thermodynamics, we refer to the first law of thermodynamics as the one for describing internal energy conservation when flow is at rest. Batchelor (1967, p. 21) describes the first law of thermodynamics as ''Work and heat are regarded as equivalent forms of energy, and the change in the internal energy of a mass of fluid *at rest* consequent on a change of state is defined, by the first law of thermodynamics, as being such as to satisfy conservation of energy when account is taken of both heat given to the fluid and work done on the fluid.'' That is, kinetic energy is not included in the first law of thermodynamics as the equilibrium state is considered; the system only includes molecular motion. The familiar thermal energy conservation equation for the atmosphere describes internal energy changes of a system within a finite volume as a result of net heating/cooling or thermal forcing, and is derived based on the first law of thermodynamics (e.g., Feynman et al. 1963; Batchelor 1967; Fleagle and Businger 1972; Gill 1982).

In a fluid system that is characterized with flow stratification and motion under the influence of gravity, conservation of energy studies the total energy including kinetic, internal (can be expressed as thermal), and potential energy (e.g., Fleagle and Businger 1972). To distinguish it from other conservation laws, we refer to conservation of energy for this type of flow as total energy conservation, which is the same as the total energy equation [Eq. (4.7.5) in Gill (1982)]. Total energy conservation describes the balance between the total energy change of the system and the rate of the net mechanical work done to the system and thermal forcing added to the system. Therefore, total energy conservation provides a constraint for changes of the sum of the thermal, kinetic, and potential energy conservation in the atmosphere. Total energy conservation has also been called the first law of thermodynamics in the literature (e.g., Bennett and Myers 1962; Balmer 2010) or simply conservation of energy (e.g., Fleagle and Businger 1972; Kuo 2005).

Theoretically, the thermal energy conservation equation can be derived as the residual balance between total energy conservation and kinetic energy conservation as demonstrated in, for example, Kuo (2005). We extend the traditional derivation of thermal energy conservation in engineering textbooks, and derive the thermal energy balance based on the physics principles of total energy conservation and momentum conservation for the atmosphere, ideal gas law, and mass conservation (section 2). Application of mass conservation explains density fluxes as a result of air thermal expansion/compression for the incompressible atmosphere, as incompressibility is associated with the air volume change with pressure under a constant temperature (American Meteorological Society 2018). Because vertical air density changes strongly impact potential energy changes, while potential energy changes are associated with kinetic energy changes, thermal energy conservation derived with the constraint of total energy conservation has to include this potential energy change as well. For this kind of nonequilibrium system, the first law of thermodynamics valid for an equilibrium system could not be applied. The resulting interaction between kinetic and thermal energy changes is different from the energy conversion between thermal and kinetic energy at a point as a result of high velocities and viscous energy dissipation such as shock waves and deceleration of a fluid approaching a subsonic stagnation point (e.g., Kays 1966). We then use observations to confirm the role of potential energy changes in explaining the diurnal variations of air temperature (section 4) based on the derived thermal energy conservation equation for the turbulent atmosphere (section 3). A summary is presented in section 5.

2. Conservation equations of total, kinetic, and thermal energy

Mathematical derivatives are commonly used to describe changes of physical variables within an infinitesimally small volume. However, following the concept of mathematical limits, such as when spatial intervals $\delta x, \delta y, \delta z \to 0$, fluid motions may not exist but only molecular diffusion. To describe the physical world, we focus on a system of a control volume that is large enough to have all components of total energy and is small enough to be described by mathematical derivatives in this study.

a. Total energy conservation

Following total energy conservation in the literature (e.g., Bennett and Myers 1962; Fleagle and Businger 1972), total energy conservation for a system of a finite volume with a constant air density ρ can be expressed as

$$\rho \frac{dE_t}{dt} = Q + F_m. \tag{1}$$

In Eq. (1), t in the dominator is the time, $d/dt = \partial/\partial t + V\partial/\partial x + w\partial/\partial z$ (V and w are the horizontal and the vertical wind speeds, respectively), E_t is the specific total energy, Q represents the rate of net heat added to the system or diabatic thermal forcing (for changing energy) such as molecular thermal conduction, and F_m is the rate of mechanical work done by the surroundings to the system. The specific total energy E_t in a geophysical fluid, such as the atmosphere where gravity plays an important role in flow motion, is the sum of the specific internal energy E_i, the specific kinetic energy $E_k = (V^2 + w^2)/2$, and the specific potential energy $E_p = zg$ (g and z are the gravity acceleration constant and the height above the surface); that is,

$$E_t = E_i + E_k + E_p. \tag{2}$$

Total energy conservation ($\mathrm{W\,m^{-2}}$) expressed in Eq. (1) reflects the balance between total energy changes or the rate of total energy inside the system on the left-hand side (lhs) and the net heating or diabatic thermal forcing and the rate of mechanical work done to the system on the right-hand side (rhs).

The rate of the mechanic work F_m consists of the rates of the work done by pressure gradients $-\nabla \cdot (\mathbf{V}p)$ ($\mathbf{V}$ is the wind vector and p is the external or environmental pressure on the boundary of the system) and by the viscous stress related to the rate of angular deformation done to the system ε (e.g., Kuo 2005); that is,

$$F_m = -\nabla \cdot (\mathbf{V}p) + \varepsilon = -\frac{\partial (Vp)}{\partial x} - \frac{\partial (wp)}{\partial z} + \varepsilon, \tag{3}$$

$$\varepsilon = \frac{\partial \sigma_{xx} V}{\partial x} + \frac{\partial \sigma_{zx} V}{\partial z} + \frac{\partial \sigma_{xz} w}{\partial x} + \frac{\partial \sigma_{zz} w}{\partial z}, \tag{4}$$

$$\sigma_{xx} = \mu\left(2\frac{\partial V}{\partial x} - \frac{2}{3}\nabla \cdot \mathbf{V}\right), \tag{5}$$

$$\sigma_{xz} = \sigma_{zx} = \mu\left(\frac{\partial w}{\partial x} + \frac{\partial V}{\partial z}\right), \quad \text{and} \tag{6}$$

$$\sigma_{zz} = \mu\left(2\frac{\partial w}{\partial z} - \frac{2}{3}\nabla \cdot \mathbf{V}\right). \tag{7}$$

In Eqs. (4)–(7), σ_{ij} is the viscous stress between the i and j directions, μ is the dynamic viscosity, and $\nabla \cdot \mathbf{V} = \partial V/\partial x + \partial w/\partial z$. For $i = j$, ε represents the normal stress; for $i \neq j$, ε represents the tangential stress.

In the atmosphere, the net heating/cooling Q in the atmosphere can come from vertical divergence of the atmospheric radiation and latent heat from water condensation, as well as molecular diffusion. Near the heated/cooled ground surface, molecular diffusion between the solid surface and the air above leads to air temperature changes. Based on the ideal gas law, $p = \rho RT$ (T is the air temperature and R is the gas constant for dry air, for which the influence of water vapor on R can be expressed in terms of the virtual temperature), air temperature changes can lead to air density changes as $\delta\rho/\rho \approx -\delta T/T$, when the background air pressure is relatively steady. Meanwhile air density changes are constrained by mass conservation,

$$\frac{d\rho}{dt} = -\rho\nabla \cdot \mathbf{V}, \tag{8}$$

which can also be expressed as

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho\mathbf{V}). \tag{9}$$

That is, an air temperature increase (decrease) leads to an air density decrease (increase) as a result of air thermal expansion (compression) even though the atmosphere is approximately incompressible. In other words, both compressibility and thermal expansion/compression can lead to $\nabla \cdot \mathbf{V} \neq 0$; here, we consider the physical processes of air thermal expansion/compression associated with $\nabla \cdot \mathbf{V} \neq 0$, as the atmospheric incompressibility is clearly demonstrated in its compressibility factor of about 1 (Green and Perry 2007) and is indirectly demonstrated in observations when atmospheric heat is effectively transferred by turbulent mixing (e.g., Sun et al. 1995; Vickers and Mahrt 2006).

Over the heated ground surface, the air density of the heated air through molecular diffusion would be less than that of the unheated air above, resulting in positive buoyancy and upward air movement, or negative vertical density fluxes. The energy for the generation of the negative vertical density flux is obtained from the air thermal expansion as a result of the thermal forcing Q. When the surface is cooled through longwave radiation, high-density air is generated from air thermal compression as the air is cooled through molecular diffusion near the surface. As a result, the air density decreases with height, and the air is stably stratified. When air motions are generated by F_m in the viscous atmosphere, vertical motions would lead to positive vertical density fluxes (Fig. 1). The positive vertical density flux enhances the potential energy of the system at the expense of the work from F_m.

In both surface heating and cooling situations described above, the vertical air density flux is associated with the external forcings of the system—Q alone for the surface heating case, and both Q and F_m for the surface cooling case. To account for the total energy change in these situations, Eq. (1) needs to include the energy change as a result of the air density change as well.

Because vertical density changes are much larger than horizontal density changes, especially in the nearly horizontally homogeneous atmosphere, the major impact of density variations on energy changes is potential energy; thus, potential energy changes associated with thermal expansion/compression as a result of the

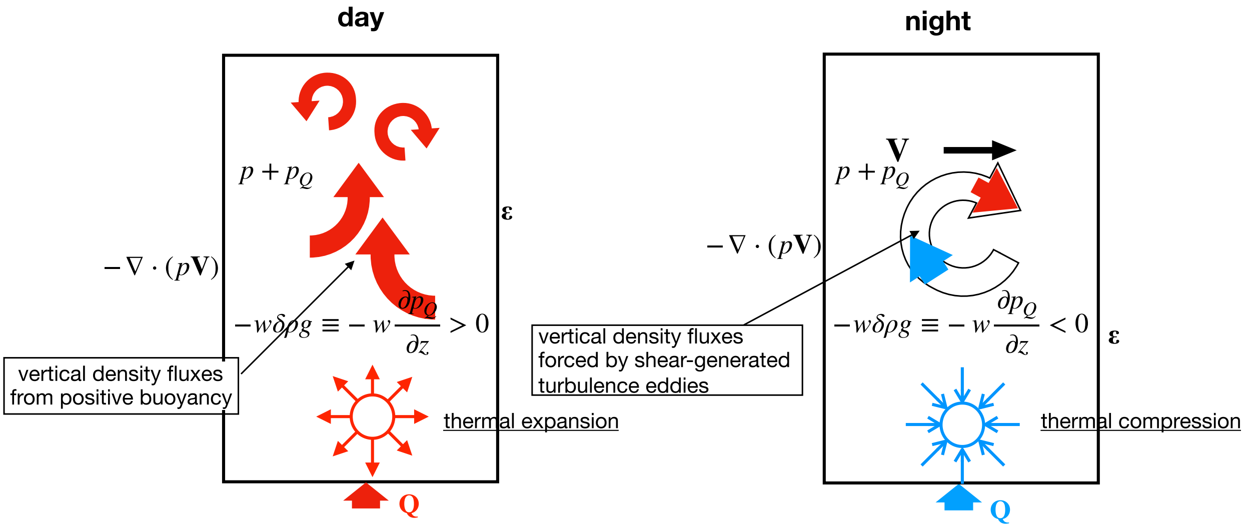

FIG. 1. Schematic showing the connection between the external thermal forcing Q and kinetic energy changes through vertical density fluxes in potential energy changes $-w\delta\rho g$ (equivalent to the work done by the nonhydrostatic pressure perturbation $-w\partial p_Q/\partial z$) generated by (left) positive buoyancy associated with air thermal expansion during the daytime and (right) shear-generated vortices at night where the vertical density distribution is contributed to by thermal compression. The external mechanical forcing to the system is $-\nabla \cdot (p\mathbf{V})$ and ε. Note that although the external thermal forcing Q is at the bottom of the system, its impact on the system can be transferred into the system through vertical density fluxes.

thermal energy transfer from Q need to be included in the total energy conservation equation [Eq. (1)]. The potential energy change associated with the vertical density fluxes as a result of thermal expansion/compression can be expressed as

$$zg\frac{\partial \rho}{\partial t} \approx zg\frac{\partial (w\rho)}{\partial z} \approx -w\delta\rho g, \qquad (10)$$

where $\delta\rho \approx z\partial\rho/\partial z$ and $w\delta\rho$ represents vertical density fluxes. Thus, total energy conservation in the atmosphere with consideration of air thermal expansion/compression would be approximated as

$$-w\delta\rho g + \rho\frac{dE_t}{dt} = Q + F_m. \qquad (11)$$

In the atmosphere, molecular motions are responsible for heat transfer in the surface viscous sublayer adjacent to the ground, where the dramatic air thermal expansion/compression occurs. Above it, turbulent mixing is much more effective in transferring heat than molecular diffusions. Because of the effective turbulent mixing above the surface viscous sublayer and its contribution to vertical density fluxes, the consequence of the thermal expansion/compression as a result of thermal energy transfer at the surface can impact air flows above the viscous sublayer where local thermal expansion/compression is relatively small.

Although we use the air heating/cooling at the surface as the examples for providing diabatic thermal forcing Q into the system, physically, Eq. (11) captures the potential energy change as a result of density fluxes generated by air thermal expansion/compression in general based on the ideal gas law and mass conservation. In the atmosphere, water phase changes and radiation of clouds can also provide similar diabatic heating/cooling sources; similar physical processes can occur. That is, vertical density fluxes can travel to a distance where local Q is negligibly small such as buoyancy fluxes under convective conditions.

b. *Kinetic energy conservation*

Inside the system, the familiar kinetic energy conservation equation with a constant air density can be derived based on momentum conservation (see the first section of the appendix) as

$$\rho\frac{dE_k}{dt} = -\mathbf{V}\cdot\nabla p - \rho w g + \varepsilon_k, \qquad (12)$$

where ε_k is the rate of dissipation of mechanical energy due to viscosity (Batchelor 1967):

$$\varepsilon_k = V\left(\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{zx}}{\partial z}\right) + w\left(\frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{zz}}{\partial z}\right). \qquad (13)$$

Because ε_k is responsible for energy cascades and dissipation heating (e.g., Garratt 1992), ε_k is negative in the atmosphere.

The kinetic energy conservation equation [Eq. (12)] reveals that kinetic energy changes are derived through the work done by mechanical forcings of the pressure gradients $-\mathbf{V}\cdot\nabla p$, viscous stress work ε_k, and the gravity body force $-\rho wg$, which is essentially the negative potential energy change. Specifically, $-V\partial p/\partial x$ contributes to the kinetic energy change associated with horizontal wind speed changes $[\rho d(V^2/2)/dt]$, and $-w(\partial p/\partial z+\rho g)$ contributes to the kinetic energy change associated with vertical wind speed changes $[\rho d(w^2/2)/dt]$ (see the first section of the appendix). The negative potential energy change $-\rho wg$ and the rate of the vertical pressure gradient $-w\partial p/\partial z$ can balance each other if the system is hydrostatically balanced ($\partial p/\partial z=-\rho g$); only the nonhydrostatic pressure gradient part, $-w(\partial p/\partial z+\rho g)\neq 0$, contributes to kinetic energy changes. As shown in the appendix's first section, the Coriolis force leads to vertical motions through turning horizontal motions or vice versa and does not change the kinetic energy of the system. Therefore, the work done by the nonhydrostatic pressure forcing is the only physical mechanism for increasing kinetic energy through vertical motions; the work related to air viscosity only reduces the mean kinetic energy. Overall, the kinetic energy conservation equation [Eq. (12)] describes how kinetic energy with an approximately invariant air density can be increased or reduced mechanically but not where energy for changing the kinetic energy comes from and how kinetic energy changes are related to environmental mechanical and thermal forcings.

Once the air density varies, the potential energy change, $-w\delta\rho g$, as in Eq. (11), also impacts kinetic energy changes. Thus, the kinetic energy conservation equation with consideration of the air density change is

$$\begin{aligned}\left(\rho\frac{dE_k}{dt}\right)^Q &\equiv -w\delta\rho g+\rho\frac{dE_k}{dt}\\ &= -\mathbf{V}\cdot\nabla p - w\rho g\left(1+\frac{\delta\rho}{\rho}\right)+\varepsilon_k\\ &= -\mathbf{V}\cdot\nabla p - w\rho g + q_{\mathrm{NH}} + \varepsilon_k,\end{aligned}\tag{14}$$

where

$$q_{\mathrm{NH}}\equiv -w\delta\rho g.\tag{15}$$

The superscript Q in Eq. (14) is used to emphasize that Eq. (14) represents the kinetic energy conservation equation with consideration of the impacts of thermal forcing Q as well as mechanical forcing F_m on kinetic energy changes; for example, positive buoyancy ($\delta\rho<0$) enhances kinetic energy through thermal plumes. Essentially, Eq. (14) is the same as the kinetic energy conservation equation derived based on the Boussinesq approximation for momentum conservation; that is, major impacts of air density changes on the atmosphere can be approximately considered in the vertical direction only (e.g., Gill 1982; Mahrt 1986; Bannon 1996). Therefore, the consideration regarding energy transfers used in deriving Eq. (10) is essentially consistent with the Boussinesq approximation for momentum transfer.

Because potential energy changes can balance kinetic energy changes by vertical pressure gradients through the hydrostatic balance as described above, another way to understand the additional mechanical forcing q_{NH} for kinetic energy changes is that q_{NH} represents the work done by an additional vertical gradient of a pressure perturbation p_Q as a result of density and temperature variations triggered by Q. That is,

$$q_{\mathrm{NH}}=-w\delta\rho g\equiv -w\frac{\partial p_Q}{\partial z},\tag{16}$$

where

$$\frac{\partial p_Q}{\partial z}\equiv\delta\rho g.\tag{17}$$

Thus, q_{NH} represents the work done by the nonhydrostatic pressure gradient $\partial p_Q/\partial z$ as a result of diabatic heating/cooling. Because the system experiences not only mechanical forcing F_m but also thermal forcing Q, the pressure p inside the system is not the ambient pressure p but $p+p_Q$.

In the turbulent atmosphere, vertical density variations are considered in decomposing air density into mean and perturbed components, and q_{NH} is essentially included in the kinetic energy conservation equation (section 3). In engineering textbooks, such as Kuo (2005), often gravity is not considered. In that situation, the impacts of q_{NH} on energy conservation cannot be studied.

c. Thermal energy conservation

With consideration of air thermal expansion/compression and its consequent impacts on potential energy changes, the total energy conservation equation [Eq. (11)] can be expressed as

$$\left(\rho\frac{dE_k}{dt}\right)^Q+\rho\frac{dE_i}{dt}+\rho\frac{dE_g}{dt}=Q+F_m.\tag{18}$$

Substituting Eq. (14) and F_m [Eq. (3)] into Eq. (18), the internal energy conservation equation constrained by total energy conservation with consideration of air density variations is

$$\rho\frac{dE_i}{dt}=Q+\varepsilon_t-q_{\mathrm{NH}}-p\nabla\cdot\mathbf{V},\tag{19}$$

where

$$
\begin{aligned}
\varepsilon_t &\equiv \varepsilon - \varepsilon_k \\
&= \frac{\partial(\sigma_{xx}V)}{\partial z} + \frac{\partial(\sigma_{zx}V)}{\partial z} + \frac{\partial(\sigma_{xz}w)}{\partial x} + \frac{\partial(\sigma_{zz}w)}{\partial z} - \left[V\left(\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{zx}}{\partial z}\right) + w\left(\frac{\partial\sigma_{xz}}{\partial x} + \frac{\partial\sigma_{zz}}{\partial z}\right)\right] \\
&= \sigma_{xx}\frac{\partial V}{\partial x} + \sigma_{xz}\frac{\partial V}{\partial z} + \sigma_{xz}\frac{\partial w}{\partial x} + \sigma_{zz}\frac{\partial w}{\partial z}
\end{aligned}
\tag{20}
$$

is the dissipation heating associated with kinetic energy dissipation (see the second section of the appendix). The dissipation heating is sometimes expressed as thermal diffusion (e.g., Garratt 1992) or neglected in the literature. Because any viscous stress reduces large-scale air motions, ε has to be negative especially when the atmosphere consists of large coherent turbulent eddies that extend down to the surface (Sun et al. 2016). The atmospheric viscous stress ε is responsible for energy cascades ε_k and the energy dissipation to heat ε_t. Because both ε and ε_k are negative and ε_t is always positive, $|\varepsilon_k|$ has to be larger than $|\varepsilon|$. The dissipation heating ε_t can be important especially when the other terms in the thermal energy conservation equation [Eq. (23)] are relatively small; even $\mu \approx 1.8 \times 10^{-5}\,\mathrm{kg\,m^{-1}\,s^{-1}}$ is relatively small for air temperature of 300 K.

We now relate internal energy to thermal energy inside the system. Using the relationship between specific enthalpy h and E_i (Kuo 2005), dE_i/dt within the system can be expressed as

$$
\frac{dE_i}{dt} = \frac{dh}{dt} - \frac{1}{\rho}\frac{dp}{dt} + \frac{p}{\rho^2}\frac{d\rho}{dt} = c_p\frac{dT}{dt} - \frac{1}{\rho}\frac{dp}{dt} - \frac{p}{\rho}\nabla\cdot\mathbf{V}, \tag{21}
$$

where c_p is the specific heat for the air under constant pressure and mass conservation [Eq. (8)] is used. Using the definition of potential temperature,[1] $\theta = T(1000/p)^{R/c_p}$, and the ideal gas law, we have

$$
c_p\frac{T}{\theta}\frac{d\theta}{dt} = c_p\frac{dT}{dt} - \frac{1}{\rho}\frac{dp}{dt}. \tag{22}
$$

Substituting Eqs. (21) and (22) into Eq. (19), the thermal energy conservation balance can be derived as

$$
\rho c_p\frac{T}{\theta}\frac{d\theta}{dt} = Q + \varepsilon_t - q_{\mathrm{NH}}. \tag{23}
$$

Fundamentally, the thermal energy conservation equation [Eq. (23)] is derived as the residual energy balance between the total energy conservation equation [Eq. (18)] and the kinetic energy conservation equation [Eq. (14)]. Because total energy conservation includes the impacts of thermal expansion/compression on energy changes, essentially the derived thermal energy balance [Eq. (23)] also includes the impacts of thermal expansion/compression on internal energy changes. Because the additional mechanic forcing q_{NH} is internally generated by vertical density fluxes associated with Q, and is not an external forcing for total energy changes, its appearance in the kinetic energy conservation equation has to balance its appearance in the thermal energy conservation equation. Thus, a positive q_{NH} in the kinetic energy equation has to balance a negative q_{NH} in the thermal energy equation; that is, the amount of the kinetic energy increase associated with a positive q_{NH} has to balance the same amount of the thermal energy decrease associated with the negative q_{NH}. The derived thermal energy conservation equation [Eq. (23)] reflects how changes in thermal and kinetic energy within the system are connected through constraint of total energy conservation. If part of the rate of the environment thermal forcing is used to change kinetic energy through air density changes, there would be a lower rate of the environment thermal forcing for changing thermal energy, as the total amount of thermal and kinetic energy changes is constrained by total energy conservation. Because vertical density fluxes are related to nonhydrostatic pressure gradient work leading to both kinetic and thermal energy changes, interactions between kinetic and thermal energy changes reflect the atmosphere self-adjustment process toward a new state of the hydrostatic balance through interactions between kinetic and thermal energy exchanges. If the nonhydrostatic pressure perturbation is continuously generated by vertical density fluxes associated with diabatic heating/cooling somewhere in the atmosphere, q_{NH} would be nonzero until its generation process ceases.

The derived thermal energy conservation equation clearly demonstrates different balance equations between temperature and other scalars such as atmospheric compositions. Because heat transfer represents energy transfer, it is capable of changing kinetic energy while concentration changes of atmospheric compositions cannot unless the concentration change can lead to potential energy changes. Dissimilarities between temperature and water vapor have indeed been observed in

[1] With significant water vapor changes, virtual potential temperature can be used (Stull 1988).

the literature (e.g., Cava et al. 2008; Van de Boer et al. 2014; Guo et al. 2016).

d. Physical differences between the traditional and the derived energy conservation equations

In the atmosphere literature, the traditional thermal energy equation relies on the first law of thermodynamics:

$$\rho\delta E_i = \int Q\,dt + \int W\,dt, \qquad (24)$$

where W is the rate of work done to the system [Eq. (24) is the same as Eq. (1.5.2) in Batchelor (1967), except here Q and W have units of the rate of energy changes instead of the amount of energy per unit mass as in Batchelor (1967)] even through Eq. (24) requires equilibrium conditions where kinetic energy is not considered. This traditional practice is different from the approach in engineering textbooks (e.g., Kuo 2005), where conservation of total energy is explicitly considered as a basic physics principle for general fluids, instead of the first law of thermodynamics. Therefore, fundamentally, the difference is whether we consider the first law of thermodynamics, which is only valid for equilibrium conditions, or total energy conservation, which is valid for nonequilibrium conditions, as a basic principle of physics for atmospheric flows.

Batchelor (1967) combined the kinetic and the thermal energy conservation equations to derive Bernoulli's theorem for steady flow. By considering the mechanical forcing F_m to a system, he added $-p\nabla\cdot\mathbf{V}+\varepsilon_t$ on both sides of the kinetic energy conservation [Eq. (12)]. Because the term $-p\nabla\cdot\mathbf{V}+\varepsilon_t$ "represents the work done in deforming the element without change of its velocity" (Batchelor 1967, p. 152), that is $W=-p\nabla\cdot\mathbf{V}+\varepsilon_t$, he combined the first law of thermodynamics [Eq. (24)] with the kinetic energy conservation equation leading to his Eq. (3.5.1), which is essentially the total energy conservation equation. Because $-p\nabla\cdot\mathbf{V}$ associated with thermal expansion/compression is not part of the kinetic energy conservation equation, but is added to have the mechanical forcing F_m, Q does not impact the kinetic energy conservation equation in his derivation. If we ignore the impacts of thermal expansion/compression on vertical density fluxes, or potential energy changes in the atmosphere, which is equivalent to setting $q_{\mathrm{NH}}=0$ or $p_Q=0$, Eq. (23) would result in the traditional thermal energy conservation equation:

$$\rho c_p \frac{T}{\theta}\frac{d\theta}{dt} = Q + \varepsilon_t. \qquad (25)$$

Similar to Batchelor (1967), Gill's (1982) work also resulted in total energy conservation [his Eq. (4.7.3)] by adding the extra expansion/compression term (without considering ε_t though) in the kinetic energy conservation equation [his Eq. (4.6.1)], where he actually considered pressure perturbation associated with density perturbation. To cancel out the thermal expansion/compression term added to the kinetic energy and the work term in the first law of thermodynamics, he has to ignore the pressure perturbation, which is again equivalent to assuming $p_Q=0$; that is, $q_{\mathrm{NH}}=0$.

Without considering vertical density transfer as a consequence of thermal expansion/compression on potential energy changes, total energy also appears to be conserved; however, the important physical connections between thermal expansion/compression and potential energy changes and interactions between kinetic and thermal energy changes through potential energy changes are not accounted for. Because of the familiarity of the Boussinesq approximation in the atmosphere community, impacts of the work through vertical density fluxes on kinetic energy changes can be accepted relatively easily. However, it is difficult to understand the extra term q_{NH} in thermal energy conservation without understanding the constraint of total energy conservation. That is, if we recognize the impacts of vertical density fluxes in changing potential energy, which in turn impacts kinetic energy changes, we have to include the same term with the opposite sign in the thermal energy conservation equation to keep total energy conserved. The different physics between the traditional and the derived thermal energy conservation equations [Eqs. (23) and (25)] is summarized schematically in Fig. 2.

The magnitude of the vertical density fluxes on potential energy changes or the magnitude of the pressure perturbation p_Q may be relatively small in comparison with the environmental pressure gradient forcing on kinetic energy changes especially near the surface where vertical air motions are constrained by the surface, but it can have the same order of magnitude as temporal variations of air temperature. Different from ε_t, which is always positive, q_{NH} can be either positive such as during the daytime or negative such as at night. Ignoring the influence of q_{NH} in thermal energy conservation can lead to systematic biases of estimating air temperature changes, that is, an overestimate of the air temperature increase when $q_{\mathrm{NH}}>0$ and an overestimate of the air temperature decrease when $q_{\mathrm{NH}}<0$.

3. Energy conservation equations in the turbulent atmosphere

In this section, we derive the kinetic energy conservation equation [Eq. (12)], where density variations are explicitly included through turbulence perturbations, and the derived thermal energy conservation equation

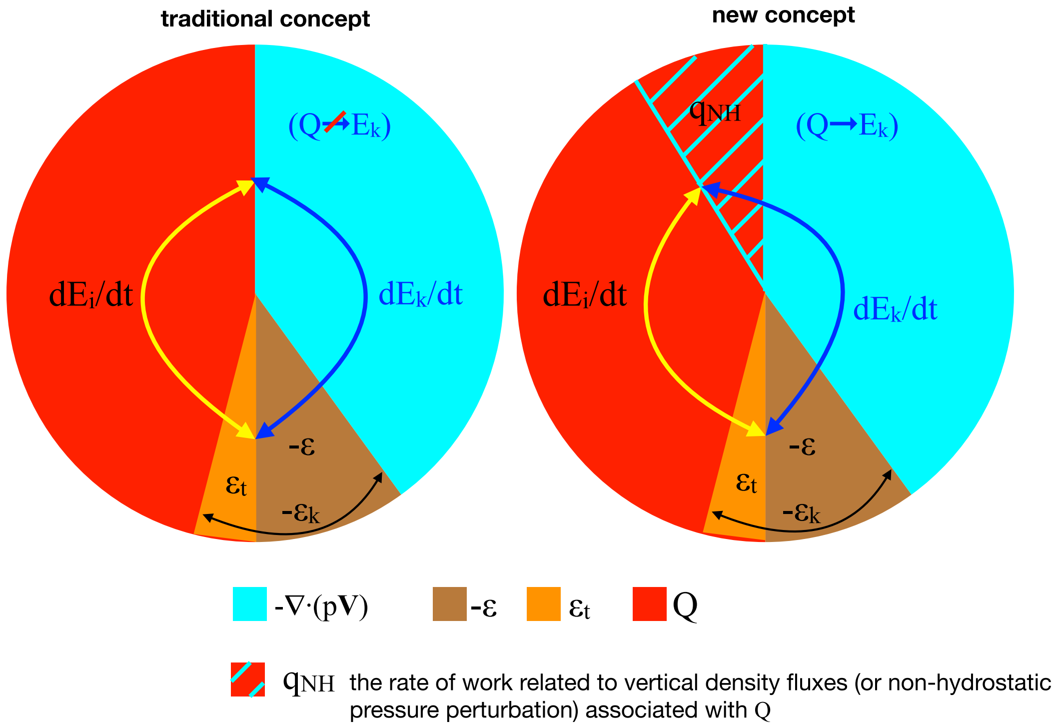

FIG. 2. Schematic illustration of the differences between the traditional and the new concepts of kinetic E_k and internal energy E_i conservation in terms of total energy conservation for a system experiencing both the external thermal forcing $Q > 0$ and the external mechanical work $-\nabla\cdot(p\mathbf{V}) + \varepsilon$ ($\mathbf{V}$, wind vector; p, external pressure; ε, the viscous deformation stress to the system). For the atmosphere, kinetic energy changes are traditionally considered to result from the mechanical forcing $-\nabla\cdot(p\mathbf{V}) + \varepsilon_k$ only, while observations indicate that part of Q is used for thermal expansion/compression, leading to vertical density fluxes and potential energy changes, q_{NH}, which contribute to kinetic energy changes as well. Recognizing the contribution of q_{NH} to kinetic energy changes, internal (or thermal) energy changes are forced by $Q - q_{NH}$, instead of Q, and $\varepsilon_t = \varepsilon - \varepsilon_k$ to satisfy total energy conservation.

[Eq. (23)] in the turbulent atmosphere. We use the traditional practice of decomposing each variable ϕ into the Reynolds-averaged mean value $\overline{\phi}$ and the perturbation $\phi' = \overline{\phi} - \phi$ as demonstrated in, for example, Stull (1988). We then examine the kinetic and the derived thermal energy balance equations up to second-order moments (terms on the order of ϕ'^2); the detailed derivations are given in the third section of the appendix. All of the other second-order-moments balance equations related to the derived thermal energy conservation equation, such as for temperature variances $\overline{\theta'^2}$ and turbulent heat fluxes $\overline{w'\theta'}$, are given later in the third section of the appendix.

With the traditional assumptions used for the turbulent atmosphere as in Stull (1988), 1) $\overline{w} \ll \overline{V}$, 2) negligibly small terms of higher-than-second-order moments, 3) horizontal homogeneity within the system ($\overline{V'\phi'} \approx 0$ and $\partial\phi/\partial x \approx 0$) not the external horizontal pressure gradient $\partial\overline{p}/\partial x$, and 4) the hydrostatic pressure balance for the mean flow ($\partial\overline{p}/\partial z = -\overline{\rho}g$), we Reynolds average the kinetic and thermal energy balance equations. By applying the Reynolds averaging to Eq. (12), the term $-w\delta\rho g$ and $\overline{p}$ in $\rho dE_k/dt$ would be included as in Eq. (14); thus, we use Reynolds averaging of the kinetic energy balance in Eq. (12) (see the third section of the appendix):

$$\overline{\rho}\left(\frac{\partial E_M}{\partial t} + \frac{\partial e}{\partial t}\right) = -\overline{V}\frac{\partial\overline{p}}{\partial x} - \overline{\rho}\frac{\partial(\overline{V}\,\overline{w'V'})}{\partial z} + \overline{q}_{NH} + \overline{\varepsilon}_k, \qquad (26)$$

where

$$E_M \equiv \frac{1}{2}(\overline{V}^2 + \overline{w}^2) \approx \frac{1}{2}\overline{V}^2, \qquad (27)$$

$$e \equiv \frac{1}{2}(\overline{V'^2} + \overline{w'^2}), \qquad (28)$$

$$\overline{q}_{NH} = \overline{\rho}\frac{g}{\overline{\theta}}\overline{w'\theta'} - \frac{\partial\overline{w'p'}}{\partial z}, \quad \text{and} \qquad (29)$$

$$\overline{\varepsilon}_k \approx \mu\left(\overline{V}\frac{\partial^2\overline{V}}{\partial z^2} + \overline{V'\frac{\partial^2 V'}{\partial z^2}} + \overline{w'\frac{\partial^2 w'}{\partial z^2}}\right). \qquad (30)$$

Here, kinetic energy in the turbulent atmosphere is decomposed into kinetic energy for mean motion (MKE) E_M and TKE for turbulent motion e. We keep both MKE and TKE in the kinetic energy conservation equation because of interactions between turbulent and mean flows [the second term on the rhs of Eq. (26)]. The mechanical energy dissipation rate $\overline{\varepsilon}_k$ in Eq. (30) is the work done by the shear stress associated with mean motion [the first term on the rhs of Eq. (30)] as well as turbulent motion [the remaining two terms on the rhs of Eq. (30)] to the considered volume. It is clear that in the turbulent atmosphere, $\overline{q}_{\rm NH}$ is generated by vertical density fluxes associated with both heat and pressure transfers [Eq. (29)].

Following the same procedure, the Reynolds-averaged new thermal energy balance [Eq. (23)] for the turbulent atmosphere (see the third section of the appendix) is

$$\left(\frac{\partial\overline{\theta}}{\partial t}+\frac{\partial\overline{w'\theta'}}{\partial z}\right)=\frac{\overline{\theta}}{c_p\overline{\rho}\,\overline{T}}(\overline{Q}-\overline{q}_{\rm NH}+\overline{\varepsilon}_t), \qquad (31)$$

where

$$\begin{aligned}\overline{\varepsilon}_t&=\overline{\varepsilon}-\overline{\varepsilon}_k\\ &=\mu\left[\left(\frac{\partial\overline{V}}{\partial z}\right)^2+\overline{\left(\frac{\partial V'}{\partial z}\right)^2}+2\overline{\left(\frac{\partial w'}{\partial z}\right)^2}\right]. \qquad (32)\end{aligned}$$

Without $\overline{q}_{\rm NH}$, Eq. (31) would be the traditional thermal energy conservation equation for the turbulent atmosphere used in the literature (e.g., Garratt 1992). Different from Reynolds averaging the kinetic energy balance [Eq. (12)], the extra term $q_{\rm NH}$ cannot be obtained by Reynolds averaging the traditional thermal energy balance [Eq. (25)], but can be obtained from the residual balance between the Reynolds-averaged total energy balance [Eq. (1)] and the Reynolds-averaged kinetic energy balance to ensure total energy conservation.

We now discuss interactions between the kinetic and thermal energy changes in the turbulent atmosphere. Turbulent motion in the atmosphere can be generated either by wind shear or positive buoyancy. Turbulence intensity measured by TKE depends not only on the energy exchange between TKE and MKE [the second term on the rhs of Eq. (26)] but also on the rate of the work associated with the vertical density fluxes $\overline{q}_{\rm NH}$, which either enhances or reduces TKE. In the literature, the impact of $\overline{q}_{\rm NH}$ on TKE is commonly split as turbulent buoyancy generation $\overline{\rho}(g/\overline{\theta})\overline{w'\theta'}$ and the TKE transport $-\partial\overline{w'p'}/\partial z$. The connection between TKE and thermal energy is traditionally interpreted through $\overline{\rho}(g/\overline{\theta})\overline{w'\theta'}$ in kinetic energy and $\partial\overline{w'\theta'}/\partial z$ in the traditional thermal energy conservation equation. This explanation may seem to be reasonable; however, $\partial\overline{w'\theta'}/\partial z$ is part of the thermal energy changes, and there is no corresponding term $\overline{\rho}(g/\overline{\theta})\overline{w'\theta'}$ in the traditional thermal energy conservation equation. Besides, if $\overline{w'\theta'}$ from $\partial\overline{w'\theta'}/\partial z$ contributes to TKE changes, there is no additional constraint condition on quantifying the partition of $\overline{w'\theta'}$ between changing thermal energy and changing TKE. In addition, physically the impact of thermal energy on TKE is through vertical air density fluxes, which are related to both temperature and pressure fluxes. The traditional thermal energy conservation equation fails to include any impact of pressure changes associated with Q on thermal energy changes. As a result, the traditional thermal energy balance does not satisfactorily explain the observed air temperature changes in the atmosphere (more in section 4).

4. Observational evidence of potential energy changes in the derived thermal energy conservation equation

Using the field dataset from the 1999 Cooperative Atmosphere–Surface Exchange Study (CASES-99), which is described in Cuxart et al. (2002) and Sun et al. (2013, 2015, 2016) for detailed observations and data processes, we examine the role of $q_{\rm NH}$ in temporal variations of air temperature described in the derived thermal energy conservation equation. In brief, the data used here are thermocouple observations sampled at $5\,{\rm s}^{-1}$ from 0.2 to 5.9 m above the surface; 5-min block-averaged $\overline{w'\theta'}$ using sonic-anemometer data at 0.5, 1.5, 5, and 20 m sampled at $10\,{\rm s}^{-1}$; $\overline{w'p'}$ using sonic-anemometer and pressure measurements sampled at $2\,{\rm s}^{-1}$ at 1.5 and 30 m; and net radiation $R_{\rm net}$ at 2 m. As the field campaign was not designed for any detailed budget study of energy conservation, we only examine evidence of the impacts of $q_{\rm NH}$ on temporal variations of air temperature in the derived thermal energy conservation equation. Based on the traditional thermal energy conservation equation, air temperature changes are closely related to vertical heat flux variations if horizontal heat advection is negligibly small. We choose two cases where horizontal heat advection is negligibly small and vertical heat flux variations are large so that temporal air temperature variations can be easily captured: 1) the daytime of 10 October, when the daytime wind speed was smallest during the entire field campaign and the vertical convergence of heat fluxes was large, and 2) the nighttime stable period between 2100 and 2200 LST 11 October, when vertical divergence of the heat fluxes was large.

We first describe the observed vertical variations of turbulent heat flux $\overline{w'\theta'}$ near the surface during the daytime. The turbulent heat flux $\overline{w'\theta'}$ is commonly related to turbulent momentum flux, $\overline{w'V'}$, as $\overline{w'\theta'} \equiv -\theta_* u_*$, where $u_* \equiv |\overline{w'V'}|^{1/2}$. Based on Sun et al. (2013), the vertical variation of u_* with height is less than 10% between 1.5 and 5 m. Using the daytime observation of sonic anemometers from the entire CASES-99 dataset, we find that the standard deviation of potential temperature σ_θ is linearly correlated with $|\theta_*|$ as θ_* is negative during the daytime (Fig. 3b), which is also reported in Sun et al. (2012). Using the thermocouple measurements, we find that the amplitude of the daytime temporal variation of σ_θ decreases with height up to about 5–6 m and the amplitude of σ_θ is about 3 times larger at 0.2 m than at 5.9 m around noon on the weak wind day of 11 October (Fig. 4a). The rapid decrease of σ_θ with height indicates that $\overline{w'\theta'}$ decreases with height significantly below about 5 m, which is in contrast with the common believe of the approximate invariance of $\overline{w'\theta'}$ (less than 10%–20% variations in the vertical) near the surface. The decrease of $\overline{w'\theta'}$ with height is independently confirmed by the directly estimated $\overline{w'\theta'}$ using the eddy-covariance method with sonic anemometers at 0.5 and 1.5 m (Fig. 3d). Considering $\overline{w'\theta'}$ at 1.5 m in Fig. 3d was estimated from the first period of the experiment when the daily maximum $R_{\rm net}$ was relatively high (Fig. 3c) and $\overline{w'\theta'}$ at 0.5 m was estimated during the second period of the experiment when the daily maximum $R_{\rm net}$ was relatively low, the vertical difference of $\overline{w'\theta'}$ between 1.5 and 0.5 m for a given day would be larger than the vertical difference of $\overline{w'\theta'}$ between the two levels shown in Fig. 3d.

We then examine the phase relationship between the temporal variation of air temperature and the vertical convergence of turbulent heat fluxes on 10 October, which should be in phase if the traditional thermal energy conservation equation [Eq. (31) with zero rhs] is valid. The close correlations between the variations of $R_{\rm net}$, TKE, and the standard deviations of w, σ_w (Figs. 4a,b), and $\overline{w'\theta'}$ (Fig. 4f) indicate that turbulence is mainly generated by positive buoyancy from the heated surface when the wind speed is steadily weak (Fig. 4d). Because the largest vertical decrease of σ_θ is around noon (Fig. 4c), the largest vertical convergence of turbulent heat fluxes should be around noon for this day. However, the observed largest temporal increase in air temperature below 5.9 m happens around 0800 LST, right at the time when the significant increase of $\overline{w'\theta'}$ begins (Fig. 4e). The inconsistency between the temporal variations of the air temperature and the vertical convergence of $\overline{w'\theta'}$ suggests that the traditional thermal energy balance is not valid.

We then examine the contribution of vertical density fluxes $\overline{q}_{\rm NH}$ [Eq. (29)] to the increase in air temperature for this day. We find that the values of $\partial\overline{w'p'}/\partial z$ based on the observations of $\overline{w'p'}$ at 1.5 and 30 m are negative and also follow the daytime variation of $R_{\rm net}$ (Fig. 4f), which is consistent with the observations in Högström (1990). Thus, both $(\overline{\rho}g/\overline{\theta})\overline{w'\theta'}$ and $-\partial\overline{w'p'}/\partial z$ in $\overline{q}_{\rm NH}$ are positive and have similar diurnal variations (Fig. 4f). The positive $\overline{q}_{\rm NH}$ would increase the kinetic energy, which is indeed observed in the simultaneous increase of TKE and $\overline{q}_{\rm NH}$ around 0800 LST, and would reduce the temporal variation of air temperature, which is indeed shown in the sharp increase of the observed $\overline{q}_{\rm NH}$ at exactly the same time as $\partial\overline{\theta}/\partial t$ starts to decrease from its maximum value (Fig. 4). Because the diurnal variation of $\overline{w'p'}$ is observed to be maximum around noon at all the observation heights, the in-phase relationship between the rapid increase of $\overline{q}_{\rm NH}$ and the rapid decrease of $\partial\overline{\theta}/\partial t$ should not be affected by any observational error in the magnitude of $\partial\overline{w'p'}/\partial z$ because of the relatively large height difference between 1.5 and 30 m for the measurements of $\overline{w'p'}$. The observation qualitatively confirms the contribution of $\overline{q}_{\rm NH}$ to the change in thermal energy.

We now investigate the impacts of $\overline{q}_{\rm NH}$ on nighttime air temperature changes between 2100 and 2200 LST on the night of 11 October when the heat flux divergence is relatively large. When the net radiation starts to decrease in the afternoon, less heat is transferred from the heated surface to $\overline{q}_{\rm NH}$, as shown in the decreases of both $(\overline{\rho}g/\overline{\theta})\overline{w'\theta'}$ and $-\partial\overline{w'p'}/\partial z$ in Fig. 4f. Because of the decreasing downward solar radiation during the afternoon while the air is still warm, the stable layer near the surface gradually develops. The available thermal forcing for changing the thermal energy gradually becomes negative, leading to a decrease in air temperature during the afternoon. At night, the air temperature adjacent to the surface decreases as a result of molecular thermal conduction from the radiatively cooled surface. When wind speed near the surface increases (Fig. 5a), wind shear due to the wind speed increase with height generates turbulence. Turbulent mixing transfers cold air upward and warm air downward, leading to the upward density flux and the net downward turbulent heat flux (Sun et al. 2012), which is observed at 5 and 20 m during 2100–2200 LST 11 October (Fig. 5b). Because the temporal variations of air temperature from the surrounding six satellite stations at the same height within the 500 m × 500 m area occur simultaneously between 2100 and 2200 LST (not shown), there is no obvious significant temperature advection. Based on the traditional thermal energy conservation equation, the observed positive $\partial\overline{w'\theta'}/\partial z$ would lead to negative $\partial\overline{\theta}/\partial t$. However, we find that $\partial\overline{\theta}/\partial t$ is slightly positive around 6 m and near zero at 20 m during this period (Fig. 5d). Based on the derived thermal energy conservation equation, the

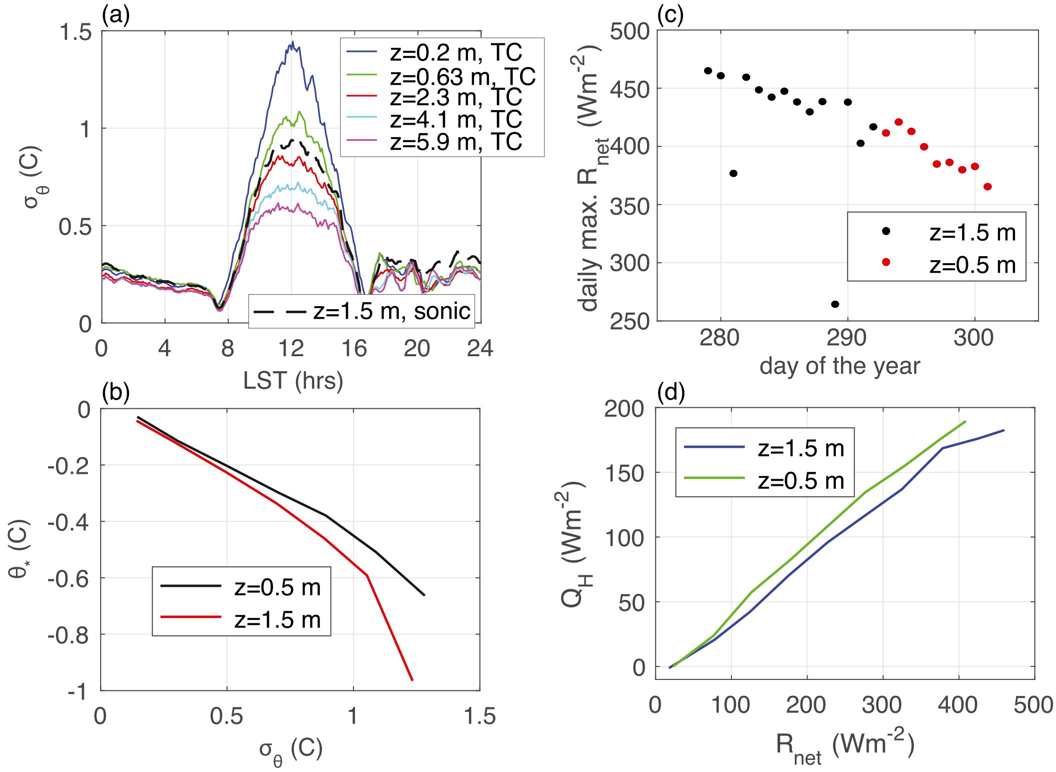

FIG. 3. (a) Diurnal variations of the standard deviation of potential temperature σ_θ within 5-min segments from the sonic anemometer measurements at 1.5 m (black dashed line) and from thermocouple (TC) measurements at the labeled heights on 11 Oct 1999. (b) The bin-averaged daytime relationships between θ_* and σ_θ at the two heights based on the entire field data. (c) The daily maximum value of net radiation $R_{\rm net}$ during the periods when the lowest sonic anemometer values were at $z = 1.5$ and 0.5 m, marked in black and red, respectively. (d) The bin-averaged daytime sensible heat flux, $Q_H = \rho c_p \overline{w'\theta'}$, as a function of net radiation at the two heights, which shows that Q_H is consistently larger at 0.5 m than at 1.5 m for a given $R_{\rm net}$.

available thermal forcing for cooling the air would be reduced as a result of the negative $\overline{q}_{\rm NH}$ from the negative $(\overline{\rho}g/\overline{\theta})\overline{w'\theta'}$ and the near-zero $-\partial\overline{w'p'}/\partial z$ (Figs. 5b,c). The negative $\overline{q}_{\rm NH}$ indicates that there is an extra positive thermal forcing for the observed positive $\partial\overline{\theta}/\partial t$. The viscous heating $\overline{\varepsilon}_t$ is too small to contribute the temperature change here considering the magnitude of the air viscosity μ and the weak wind speed associated with the stable conditions.

Examples of both the daytime and nighttime observations suggest that the traditional thermal energy conservation balance cannot explain the observed diurnal variation of air temperature. Including $\overline{q}_{\rm NH}$ in the thermal energy conservation equation could qualitatively explain the temporal variation of air temperature during the day and night. The gradual decrease of $\partial\overline{\theta}/\partial t$ from its peak value around 0800 LST as $\overline{q}_{\rm NH}$ gradually increases during the daytime suggests that the magnitude of $\overline{q}_{\rm NH}$ could be on the same order of magnitude as $\partial\overline{\theta}/\partial t$, as the vertical density flux has to be relatively small near the surface due to $w = 0$ at the surface. However, the presence of $\overline{q}_{\rm NH}$ in the derived thermal energy conservation equation is physically important in explaining the observed diurnal variation of air temperature. Quantifying the contribution of $\overline{q}_{\rm NH}$ to $\partial\overline{\theta}/\partial t$ requires better observations near the surface. As the term $\overline{q}_{\rm NH}$ depends on the vertical density fluxes and the vertical scale of turbulence eddies increases with height (e.g., Sun et al. 2016), the role of $\overline{q}_{\rm NH}$ in atmospheric thermodynamics such as cyclogenesis could be significant.

5. Summary

Applying total and kinetic energy conservation, we revisit thermal energy conservation (related to internal energy) in the atmosphere. Kinetic energy conservation is impacted not only by environment mechanical work F_m but also by potential energy changes related to vertical density fluxes resulting from accumulated thermal expansion/compression from net heating Q (diabatic thermal forcing), $q_{\rm NH}$, even though the atmosphere is approximately incompressible. The effects of thermal expansion/compression on air

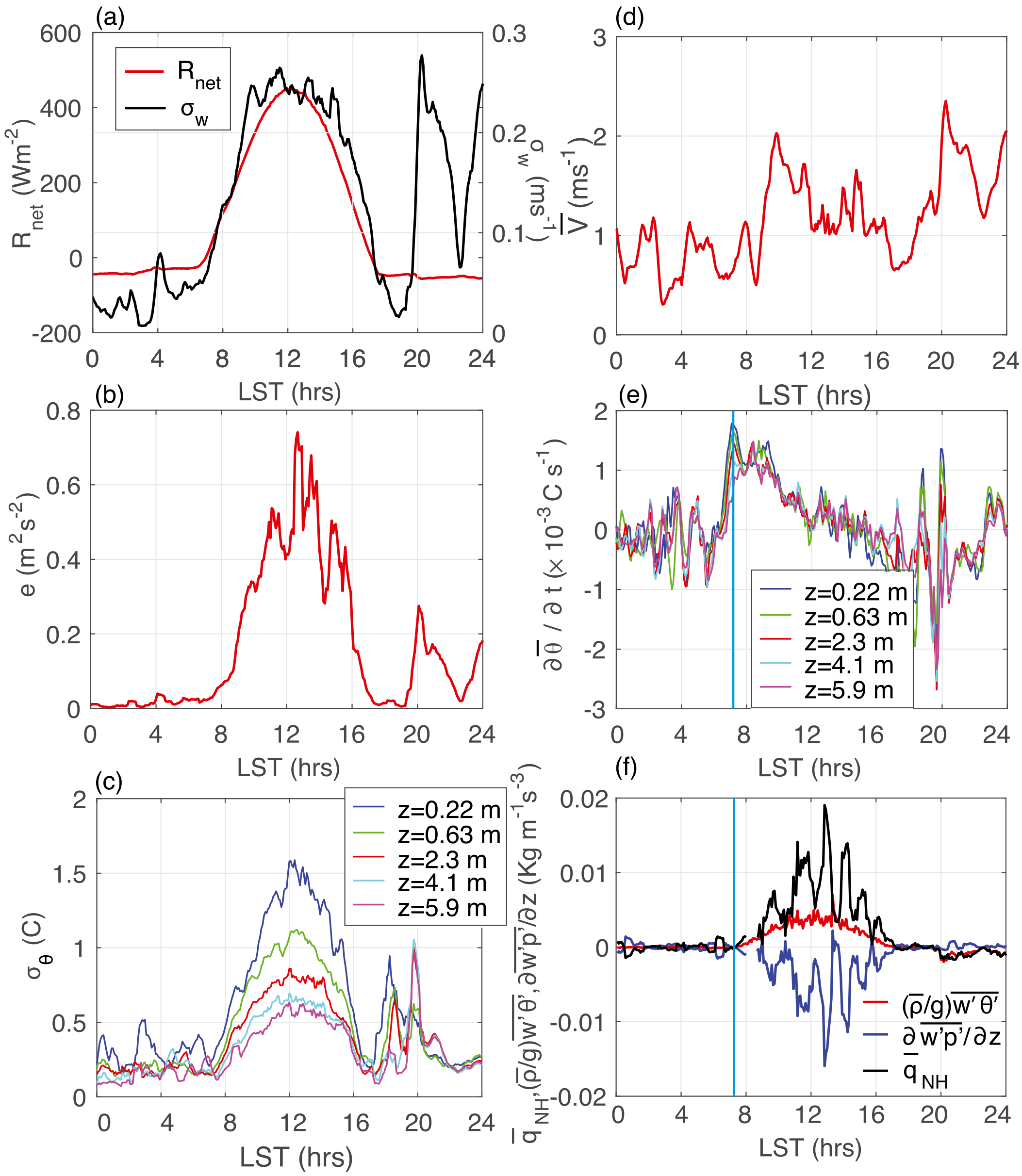

FIG. 4. Diurnal variations of (a) the net radiation R_{net} and the standard deviation of the vertical velocity σ_w from 5-min segments, where σ_w is related to the contribution of w to TKE, (b) TKE e at 1.5 m, (c) the 5-min standard deviation of the thermocouple temperature σ_θ at the labeled heights, (d) wind speed $\overline{V}$ at 5 m, (e) the temporal variation of the thermocouple temperature $\partial\overline{\theta}/\partial t$ at the labeled heights, and (f) the kinematic heat flux $(g/\overline{\theta})\overline{w'\theta'}$ at 1.5 m, $\partial\overline{w'p'}/\partial z$ based on the measurements of $\overline{w'p'}$ at 1.5 and 30 m, and $\overline{q}_{\mathrm{NH}} = (g/\overline{\theta})\overline{w'\theta'} - \partial\overline{w'p'}/\partial z$ on the steady weak wind day of 10 Oct. The vertical cyan lines in (e) and (f) mark the time when $\partial\overline{\theta}/\partial t$ starts to decrease and $\overline{q}_{\mathrm{NH}}$ starts to increase. A 25-min running mean is applied for all plots.

motions should not be confused with air compressibility as air compressibility refers to air volume changes with pressure at a constant temperature even though both lead to $\nabla \cdot \mathbf{V} \neq 0$. Vertical density fluxes can be generated by thermal expansion at a distance, or by mechanically generated vertical mixing in the stably stratified atmosphere that has been contributed to by diabatic cooling. With consideration of the impacts of q_{NH} on kinetic energy changes and the constraint of total energy conservation on the sum of the kinetic, potential, and internal energy changes, the thermal energy balance should include not only Q and dissipation heat ε_t but also q_{NH}.

The presence of q_{NH} in both kinetic and thermal energy conservation equations clearly demonstrates the

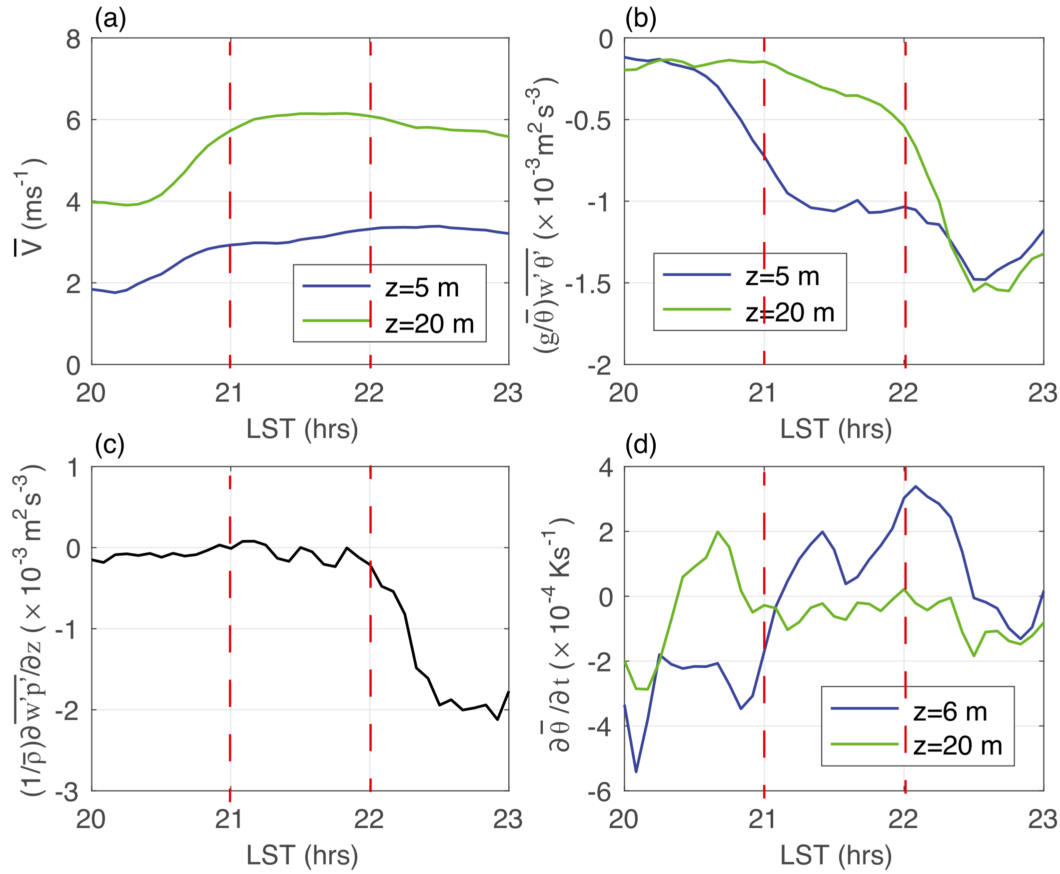

FIG. 5. (a) The wind speed $\overline{V}$, (b) $(g/\overline{\theta})\overline{w'\theta'}$, (c) $(1/\overline{\rho})\partial\overline{w'p'}/\partial z$ based on the measurements of $\overline{w'p'}$ at 1.5 and 30 m, and (d) the temporal variation of potential temperature $\partial\overline{\theta}/\partial t$ as a function of LST during the night of 11 Oct, where the period of interest is between the red dashed lines.

physical connections between kinetic and thermal energy exchanges, which are stability effects on atmospheric motions. Interactions between kinetic and thermal energy also reflect an important transition between a nonhydrostatic-pressure-balanced state and a hydrostatic-pressure-balanced state in the stratified atmosphere. The observed simultaneous increase of q_{NH} and the decrease of the temporal variation of air temperature during the daytime, as well as the observed air temperature increase with $q_{NH} < 0$ when vertical heat fluxes are divergent at night, presented in this study qualitatively confirm the suggested inclusion of q_{NH} in the thermal energy balance. As q_{NH} varies diurnally near the surface, it has systematic impacts on temporal variations of air temperature even though its magnitude near the surface could be relatively small in comparison with the horizontal pressure gradient forcing on kinetic energy changes. With strong vertical density fluxes associated with thermal expansion/compression as a result of large diabatic heating, q_{NH} could contribute significantly to air motions and thermodynamic structures.

The traditional thermal energy conservation equation for the atmosphere is guided by the first law of thermodynamics even though it is only valid for an equilibrium state for which air motions are not included. Because the first law of thermodynamics does not explicitly include air motions, except for molecular motions, the impacts of environmental mechanical and thermal forcing on a system are somewhat isolated: mechanical forcing is used for kinetic energy changes and thermal forcing is used for thermal energy changes only. Applying the first law of thermodynamics to a nonequilibrium system not only violates the required equilibrium condition, but also misses the contribution of thermal forcing to air motions. Vertical convergence/divergence of heat fluxes in the traditional thermal energy balance represents internal energy changes, not potential energy changes associated with thermal expansion/compression. Therefore, in the traditional thermal energy balance, q_{NH} is implicitly zero. Ignoring the potential energy changes associated with vertical density fluxes in both the kinetic and thermal energy conservation equations appears to satisfy total energy conservation, but misses important impacts of thermal expansion/compression on air motions and thermodynamics, and results in an unsatisfactory explanation of the observations. In practice, the impacts of vertical density variations are often considered in the momentum balance, such as the Boussinesq approximation, which is equivalent to including q_{NH} in kinetic energy conservation. Applying the traditional thermal energy balance without including q_{NH} while including q_{NH} in the kinetic energy balance would violate total energy conservation and lead to systematic biases in estimates of air temperature changes.

The derived thermal energy conservation equation also demonstrates that temperature and atmospheric compositions have different balance equations. Unlike regular scalars such as atmospheric compositions, temperature transfer is associated with energy transfer, and impacts not only thermal energy changes but also kinetic energy changes. Differences between the derived thermal energy balance and the conservation equation of atmospheric compositions may shed light on observed dissimilarities between temperature and water vapor in the literature.

The derived thermal energy conservation equation could also potentially improve our understanding of the observed atmospheric thermodynamic structures, for example, in explaining the well-observed surface energy imbalance problem, which is based on the traditional thermal energy balance. Impacts of the derived thermal energy balance on atmospheric thermodynamics could be important not only in the atmospheric boundary layer, as demonstrated in this study, but also in large-scale and mesoscale atmospheric and oceanic thermodynamics whenever vertical density fluxes prevail in space. The concept of vertical density fluxes in connecting kinetic and thermal energy changes with consideration of total energy conservation could also contribute to a better understanding of the available potential energy in the literature (e.g., Tailleux 2013). Further field and laboratory investigations into energy conservation, especially total and thermal energy conservation, are needed to quantitively verify the derived thermal energy balance. Exploration of interactions between kinetic and thermal energy changes by numerical models would require consideration of thermal expansion/compression in generating vertical density fluxes in both kinetic and thermal conservation equations because all current numerical models including high-resolution ones are based on the traditional thermal energy balance, in which thermal expansion/compression is not explicitly included to relate to air motions and atmospheric thermodynamic structures.

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APPENDIX

Derivation of Energy Conservation Equations

a. Kinetic energy conservation

For a two-dimensional flow (V and w in the directions of x and z), the horizontal and the vertical momentum balance equations for a small-volume system can be expressed as (e.g., Kuo 2005)

$$\rho\frac{dV}{dt} = -\frac{\partial p}{\partial x} + \left(\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{zx}}{\partial z}\right) = -\frac{\partial p}{\partial x} + \mu\left[\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial z^2} + \frac{1}{3}\frac{\partial}{\partial x}(\nabla\cdot\mathbf{V})\right] \quad \text{and} \tag{A1}$$

$$\rho\frac{dw}{dt} = -\frac{\partial p}{\partial z} - \rho g + \left(\frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{zz}}{\partial z}\right) = -\frac{\partial p}{\partial z} - \rho g + \mu\left[\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial z^2} + \frac{1}{3}\frac{\partial}{\partial z}(\nabla\cdot\mathbf{V})\right], \tag{A2}$$

where μ is the dynamic air viscosity and $\nabla\cdot\mathbf{V} = \partial V/\partial x + \partial w/\partial z$. Note that the above momentum balance equations implicitly assume that there is no air density variation. The equations for the horizontal and vertical contributions of kinetic energy can be derived by multiplying Eq. (A1) by V and Eq. (A2) by w as

$$\rho\frac{d(V^2/2)}{dt} = -V\frac{\partial p}{\partial x} + V\left(\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{zx}}{\partial z}\right) = -V\frac{\partial p}{\partial x} + \mu V\left[\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial z^2} + \frac{1}{3}\frac{\partial}{\partial x}(\nabla\cdot\mathbf{V})\right] \quad \text{and} \tag{A3}$$

$$\rho\frac{d(w^2/2)}{dt} = -w\left(\frac{\partial p}{\partial z} + \rho g\right) + w\left(\frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{zz}}{\partial z}\right) = -w\left(\frac{\partial p}{\partial z} + \rho g\right) + \mu w\left[\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial z^2} + \frac{1}{3}\frac{\partial}{\partial z}(\nabla\cdot\mathbf{V})\right]. \tag{A4}$$

Adding Eqs. (A3) and (A4), we have the conservation equation for kinetic energy, $E_k = 1/2(V^2 + w^2)$, as

$$\rho\frac{dE_k}{dt} = -V\frac{\partial p}{\partial x} - w\left(\frac{\partial p}{\partial z} + \rho g\right) + \varepsilon_k, \tag{A5}$$

where

$$\varepsilon_k = \left[V\left(\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xz}}{\partial z}\right) + w\left(\frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{zz}}{\partial z}\right)\right]$$
$$= \mu\left\{V\left[\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial z^2} + \frac{1}{3}\frac{\partial}{\partial x}(\nabla\cdot\mathbf{V})\right]\right.$$
$$\left. + w\left[\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial z^2} + \frac{1}{3}\frac{\partial}{\partial z}(\nabla\cdot\mathbf{V})\right]\right\} \tag{A6}$$

represents the mechanical stress work to the system or the kinetic energy dissipation ($\varepsilon_k < 0$).

With consideration of the Coriolis effect, the extra forcing for the wind acceleration in a three-dimensional flow of u, v, and w in the orthogonal directions of x, y, and z would be

$$\frac{du}{dt} = \cdots + 2\Omega_y w - 2\Omega_z v, \tag{A7}$$

$$\frac{dv}{dt} = \cdots + 2\Omega_z u - 2\Omega_x w, \quad \text{and} \tag{A8}$$

$$\frac{dw}{dt} = \cdots + 2\Omega_x v - 2\Omega_y u, \tag{A9}$$

where $\boldsymbol{\Omega} = (\Omega_x, \Omega_y, \Omega_z)$ is the angular velocity of Earth. To obtain the kinetic energy balance equation, we add Eq. (A7) multiplied by u, Eq. (A8) multiplied by v, and Eq. (A9) multiplied by w; thus, the change in total kinetic energy resulting from the Coriolis force would be

$$u(2\Omega_y w - 2\Omega_z v) + v(2\Omega_z u - 2\Omega_x w)$$
$$+ w(2\Omega_x v - 2\Omega_y u) = 0. \tag{A10}$$

That is, the Coriolis effect does not contribute to changes in kinetic energy, $(u^2 + v^2 + w^2)/2$.

b. *Work associated with viscosity*

Here, we first expand the viscous stress for total energy conservation ε. Substituting Eqs. (5)–(7) into Eq. (4), we have

$$\varepsilon = \frac{\partial \sigma_{xx}V}{\partial x} + \frac{\partial \sigma_{zx}V}{\partial z} + \frac{\partial \sigma_{xz}w}{\partial x} + \frac{\partial \sigma_{zz}w}{\partial z} = \mu\left\{V\left(\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial z^2}\right) + w\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial z^2}\right)\right.$$
$$\left. + 2\left[\left(\frac{\partial V}{\partial x}\right)^2 + \left(\frac{\partial w}{\partial z}\right)^2\right] + \left(\frac{\partial V}{\partial z} + \frac{\partial w}{\partial x}\right)^2 + \frac{1}{3}V\left(\frac{\partial \nabla\cdot\mathbf{V}}{\partial x} + w\frac{\partial \nabla\cdot\mathbf{V}}{\partial z}\right) - \frac{2}{3}(\nabla\cdot\mathbf{V})^2\right\}. \tag{A11}$$

The heating associated with the energy dissipation ε_t in Eq. (20) can be obtained by substituting Eqs. (5)–(7) into Eq. (20), or by subtracting Eq. (A6) from Eq. (A11); that is,

$$\varepsilon_t = \mu\left\{2\left[\left(\frac{\partial V}{\partial x}\right)^2 + \left(\frac{\partial w}{\partial z}\right)^2\right]\right.$$
$$\left. + \left(\frac{\partial V}{\partial z} + \frac{\partial w}{\partial x}\right)^2 - \frac{2}{3}(\nabla\cdot\mathbf{V})^2\right\}. \tag{A12}$$

The above equation for ε_t indicates that ε_t is always positive unless air expansion/compression $\nabla\cdot\mathbf{V} \neq 0$ for the approximately incompressible atmosphere is extremely large based on the discussion of the differences between air expansion/compression and air compressibility in the text.

When the work associated with the air expansion/compression is negligibly small compared to other energy transfers in ε, ε_k, and ε_t, that is, $\nabla\cdot\mathbf{V} \approx 0$ is approximately valid in Eqs. (A11), (A6), and (A12), ε, ε_k, and ε_t can be simplified as

$$\varepsilon \approx \mu\left\{V\left(\frac{\partial^2 V}{\partial x^2}+\frac{\partial^2 V}{\partial z^2}\right)+w\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial z^2}\right)+2\left[\left(\frac{\partial V}{\partial x}\right)^2+\left(\frac{\partial w}{\partial z}\right)^2\right]+\left(\frac{\partial V}{\partial z}+\frac{\partial w}{\partial x}\right)^2\right\}, \quad \text{(A13)}$$

$$\varepsilon_k \approx \mu\left[V\left(\frac{\partial^2 V}{\partial x^2}+\frac{\partial^2 V}{\partial z^2}\right)+w\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial z^2}\right)\right], \quad \text{and} \quad \text{(A14)}$$

$$\varepsilon_t \approx \mu\left\{2\left[\left(\frac{\partial V}{\partial x}\right)^2+\left(\frac{\partial w}{\partial z}\right)^2\right]+\left(\frac{\partial V}{\partial z}+\frac{\partial w}{\partial x}\right)^2\right\}. \quad \text{(A15)}$$

c. *Turbulent atmosphere*

1) Conservation equations of kinetic and thermal energy in the turbulent atmosphere

Here, we derive the conservation equations of kinetic and thermal energy for the turbulent atmosphere. Because of the effectiveness of turbulence in heat transfer in comparison with molecular thermal transfer, the air expansion/compression associated with molecular motions can be assumed to be approximately negligible (i.e., $\nabla\cdot\mathbf{V}\approx 0$ in the turbulent atmosphere). Following the traditional approach for deriving Reynolds-averaged equations as in Stull (1988), we decompose any variable ϕ in the balance equation as $\phi=\overline{\phi}+\phi'$, where $\overline{\phi}$ and ϕ' represent the Reynolds mean and turbulent components. The turbulence balance equation can be obtained by Reynolds averaging the decomposed balance equation. As practiced in the traditional derivation of any turbulence balance equation, we apply the following assumptions: 1) $\phi'/\overline{\phi}\ll 1$; 2) terms with higher-than-second-order-moment terms, for example, ϕ'^3, are negligibly small (i.e., $\phi'^3\approx 0$); 3) Reynolds-averaged horizontal components inside the considered system are much smaller than Reynolds-averaged vertical components (i.e., $\overline{V'\phi'}\ll\overline{w'\phi'}$); 4) the mean vertical motion is negligibly small (i.e., $\overline{w}\approx 0$); 5) $\partial V'/\partial x+\partial w'/\partial z\approx 0$; and 6) the mean background flow is hydrostatically balanced (i.e., $\partial\overline{p}/\partial z\approx -\overline{\rho}g$). The last assumption implies that $\overline{q}_{\rm NH}$ is entirely associated with turbulent mixing.

To obtain the Reynolds-averaged kinetic energy conservation equation [Eq. (A5)], we first Reynolds-average the decomposed dE_k/dt as

$$\overline{\frac{dE_k}{dt}}=\overline{\frac{d(\overline{V}+V')^2}{dt}}+\overline{\frac{d(\overline{w}+w')^2}{dt}}\approx\frac{D(\overline{V}^2/2)}{Dt}+\frac{D(\overline{V'^2}/2)}{Dt}+\overline{V}\left(\frac{\partial\overline{V'^2}}{\partial x}+\frac{\partial\overline{w'V'}}{\partial z}\right)+\overline{V'^2}\frac{\partial\overline{V}}{\partial x}+\overline{w'V'}\frac{\partial\overline{V}}{\partial z}$$
$$+\frac{D(\overline{w}^2/2)}{Dt}+\frac{D(\overline{w'^2}/2)}{Dt}+\overline{w}\left(\frac{\partial\overline{w'V'}}{\partial x}+\frac{\partial\overline{w'^2}}{\partial z}\right)+\overline{w'V'}\frac{\partial\overline{w}}{\partial x}+\overline{w'^2}\frac{\partial\overline{w}}{\partial z}\approx\frac{\partial E_M}{\partial t}+\frac{\partial e}{\partial t}+\frac{\partial(\overline{V}\,\overline{w'V'})}{\partial z}, \quad \text{(A16)}$$

where $E_M\equiv(1/2)(\overline{V}^2+\overline{w}^2)\approx(1/2)\overline{V}^2$ and $e\equiv(1/2)(\overline{V'^2}+\overline{w'^2})$ represent kinetic energy for MKE and TKE, respectively, and $D/Dt=\partial/\partial t+\overline{V}\partial/\partial x+\overline{w}\partial/\partial z$. We then Reynolds-average all the terms on the right-hand side of Eq. (A5) as

$$\overline{-V\frac{\partial p}{\partial x}}=-\overline{V}\frac{\partial\overline{p}}{\partial x}-\frac{\overline{V}}{\overline{\theta}}\overline{\theta'\frac{\partial p'}{\partial x}}-\overline{V'\frac{\partial p'}{\partial x}}-\frac{\overline{V'\theta'}}{\overline{\theta}}\frac{\partial\overline{p}}{\partial x}\approx-\overline{V}\frac{\partial\overline{p}}{\partial x}, \quad \text{(A17)}$$

$$\overline{q}_{\rm NH}=-\overline{(\overline{w}+w')\left[\frac{\partial(\overline{p}+p')}{\partial z}+(\overline{\rho}+\rho')g\right]}\approx\frac{\overline{\rho}g}{\overline{\theta}}\overline{w'\theta'}-\frac{\partial\overline{w'p'}}{\partial z}, \quad \text{and} \quad \text{(A18)}$$

$$\overline{\varepsilon}_k\approx\mu\left(\overline{V}\frac{\partial^2\overline{V}}{\partial z^2}+\overline{V'\frac{\partial^2 V'}{\partial z^2}}+\overline{w'\frac{\partial^2 w'}{\partial z^2}}\right). \quad \text{(A19)}$$

In Eqs. (A17) and (A18), the definitions of potential temperature $\theta=T(1000/p)^{R/c_p}$ and the ideal gas law $p=\rho RT$ are applied, such that

$$\rho'=\overline{\rho}\left(\frac{p'}{\overline{p}}-\frac{T'}{\overline{T}}\right)=\overline{\rho}\left[-\frac{\theta'}{\overline{\theta}}+\left(1+\frac{R}{c_p}\right)\frac{p'}{\overline{p}}\right]\approx\overline{\rho}\,\frac{\theta'}{\overline{\theta}}. \quad \text{(A20)}$$

In Eq. (A20), $(p'/\overline{p})(1-R/c_p)\ll\theta'/\overline{\theta}$ is also used based on the CASES-99 observations of $\theta'/\overline{\theta}\approx\sigma_\theta/\overline{\theta}\approx 1/300=3\times10^{-3}$ and $p'/\overline{p}\approx\sigma_p/\overline{p}\approx 0.02/1000=2\times10^{-5}$. Combining Eqs. (A16)–(A19), we have the Reynolds-averaged kinetic energy equation:

$$\overline{\rho}\left(\frac{\partial E_M}{\partial t}+\frac{\partial e}{\partial t}\right)=-\overline{V}\frac{\partial\overline{p}}{\partial x}-\frac{\partial\overline{V}\,\overline{w'V'}}{\partial z}+\overline{q}_{\mathrm{NH}}+\overline{\varepsilon}_k. \quad \text{(A21)}$$

Note that decomposing the kinetic energy balance equation [Eq. (A5)] contribution of density variations to kinetic energy changes is implicitly included in the decomposed ρ. Reynolds averaging the decomposed kinetic energy balance indicates that $\overline{q}_{\mathrm{NH}}$ represents a coherent contribution between w' and ρ', while the contribution of the density variations to other terms is Reynolds averaged out based on the assumptions listed for Reynolds averaging.

Following the same procedures with the same assumptions, the Reynolds-averaged lhs of the derived thermal energy conservation [Eq. (23)] is

$$c_p\overline{\rho\frac{T}{\theta}\frac{d\theta}{dt}}\approx c_p\overline{\frac{(\overline{\rho}+\rho')(\overline{T}+T')}{\overline{\theta}}\left(1+\frac{\theta'}{\overline{\theta}}\right)\frac{d(\overline{\theta}+\theta')}{dt}}$$
$$\approx\overline{\rho}c_p\frac{\overline{T}}{\overline{\theta}}\left(\frac{\partial\overline{\theta}}{\partial t}+\frac{\partial\overline{w'\theta'}}{\partial z}\right). \quad \text{(A22)}$$

Thus, the Reynolds-averaged new thermal energy conservation equation [Eq. (23)] becomes

$$\overline{\rho}c_p\frac{\overline{T}}{\overline{\theta}}\left(\frac{\partial\overline{\theta}}{\partial t}+\frac{\partial\overline{w'\theta'}}{\partial z}\right)=\overline{Q}-\overline{q}_{\mathrm{NH}}+\overline{\varepsilon}_t, \quad \text{(A23)}$$

where

$$\overline{\varepsilon}_t=\overline{\varepsilon}-\overline{\varepsilon}_k$$
$$\approx\mu\left[\left(\frac{\partial\overline{V}}{\partial z}\right)^2+\overline{\left(\frac{\partial V'}{\partial z}\right)^2}+2\overline{\left(\frac{\partial w'}{\partial z}\right)^2}\right]. \quad \text{(A24)}$$

2) BALANCE EQUATIONS FOR TEMPERATURE-RELATED VARIABLES

With all the assumptions used above, the turbulence-perturbed thermal energy equation [Eq. (23)] can be obtained by subtracting the Reynolds-averaged Eq. (23) from the decomposed Eq. (23) as

$$\frac{\overline{\rho}c_p\overline{T}}{\overline{\theta}}\left(\frac{\partial\theta'}{\partial t}+w'\frac{\partial\overline{\theta}}{\partial z}\right)\approx Q'+\varepsilon_t', \quad \text{(A25)}$$

where

$$\varepsilon_t'=2\mu\frac{\partial\overline{V}}{\partial z}\frac{\partial V'}{\partial z}\quad\text{and}\quad q_{\mathrm{NH}}'\approx 0. \quad \text{(A26)}$$

Multiplying Eq. (A25) by θ' and Reynolds averaging the equation, we have

$$\frac{\partial\overline{(\theta'^2)}/2}{\partial t}=-\overline{w'\theta'}\frac{\partial\overline{\theta}}{\partial z}+\frac{\overline{\theta}\,\overline{\theta'Q'}}{c_p\overline{\rho}\,\overline{T}}, \quad \text{(A27)}$$

where $\overline{\theta'\varepsilon_t'}\approx 0$.

The turbulence-perturbed vertical momentum conservation with all the assumptions used above is

$$\frac{\partial w'}{\partial t}=-\frac{1}{\overline{\rho}}\frac{\partial p'}{\partial z}+g\frac{\theta'}{\overline{\theta}}. \quad \text{(A28)}$$

Adding Eq. (A28) multiplied by θ' to Eq. (A25) multiplied by w', and Reynolds averaging the resulting equation, we have the balance equation for $\overline{w'\theta'}$:

$$\frac{\partial\overline{w'\theta'}}{\partial t}\approx-\overline{w'^2}\frac{\partial\overline{\theta}}{\partial z}-\frac{1}{\overline{\rho}}\overline{\theta'\frac{\partial p'}{\partial z}}+\frac{\overline{\theta'^2}g}{\overline{\theta}}+\frac{\overline{\theta}}{c_p\overline{\rho}\,\overline{T}}(\overline{w'Q'}+\overline{w'\varepsilon_t'}), \quad \text{(A29)}$$

where

$$\overline{w'\varepsilon_t'}=\overline{w'\varepsilon'}-\overline{w'\varepsilon_k'}=2\mu\frac{\partial\overline{V}}{\partial z}\frac{\partial\overline{w'V'}}{\partial z}. \quad \text{(A30)}$$

The above derivations indicate that for small turbulent perturbations, $q_{\mathrm{NH}}'\approx 0$ if we ignore third-order-moment terms. Under these conditions, the impacts of q_{NH} on the atmosphere are expected to be only important in regard to the changes in mean air temperature through $\overline{q}_{\mathrm{NH}}$ [Eq. (A23)], but less so in terms of the changes in temperature fluctuations [Eq. (A27)] and turbulent heat fluxes [Eq. (A29)].

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