

Exact Averaging of Atmospheric State and Flow Variables

ANDREW S. KOWALSKI

Departamento de Física Aplicada, Universidad de Granada, and Centro Andaluz del Medio Ambiente, Granada, Spain

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ABSTRACT

A new set of averaging rules is put forward that exactly determines the means of air temperature, mixing ratio, and velocity by incorporating weighting factors in accordance with physical conservation laws. For the temperature and velocity, respectively, the means calculated according to these rules are shown to be in accordance with the gas law and the most fundamental definition from classical mechanics. By contrast, those reckoned according to traditional arithmetic averaging rules are found to be incorrect. For studies of eddy transport, and micrometeorology in particular, such imprecisely determined averages of state and flow variables bias the perturbation variables over the entire averaging domain and thereby skew estimates of mass, heat, and momentum exchange unless appropriate adjustments (such as density corrections) are applied. The exact calculation of gas-phase averages amends this problem and is equally applicable to planetary-, synoptic-, and mesoscale averaging, as well as to climatology.

1. Introduction

The statistical and mathematical operation of averaging is essential to the atmospheric sciences and underlies most fundamental meteorological laws. Even at the smallest scales, atmospheric state and flow variables inherently involve some form of averaging, such as that realized over an instrument sensing volume or model grid cell. The bulk of gas law truly applies only to means (hereinafter the terms “average” and “mean” will be used interchangeably), since the key state variables pressure and temperature are defined by kinetic theory as *average* molecular characteristics of momentum transfer and kinetic energy, respectively (Giancoli 1984). Similarly, given the irrelevance of reckoning individual molecular velocities, atmospheric dynamics is concerned with the behavior of macroscopic means of myriad molecules. Along with its inverse process of decomposition, averaging is essential when adapting data and models to the appropriate scales of interest.

Defining the mean is the first step in describing perturbations whose transport of mass, heat, and momentum are the focus of entire subdisciplines of meteorology. In

the study of turbulence and waves at multiple scales, such perturbations are determined by subtracting, from the overall state or flow, the mean or “basic state” (Holton 1992). In such a decomposition procedure, usually carried out according to “Reynolds rules,” an inexact calculation of the mean would bias the relevant perturbation variable over the entire averaging domain. And there is evidence of such inaccuracy, like the dubious assertion derived from textbook “Reynolds averaging” that the gas law is merely approximate when applied to averages, unless certain state-variable covariance terms are included [e.g., Stull 1988, Eq. (3.3.1b)], as if the very form of the gas law were scale dependent (see section 4a). Such errors may have significant import, particularly for fields of study that rely on Reynolds rules to define transport by waves and eddies.

Boundary layer meteorology, a field heavily dependent on Reynolds averaging and decomposition procedures to define near-surface turbulent eddies, clearly suffers from a grave and persistent fault. The inability to close the surface energy budget (Foken 2008a) is a serious setback for a discipline largely devoted to assessing surface exchanges of mass, energy, and momentum. This shortcoming was apparent decades ago (Leuning et al. 1982), but its prevalence became notable (Aubinet et al. 2000; Wilson et al. 2002) once the 1997 Kyoto Protocol had spurred a vast expansion in tower-based flux measurements (Baldocchi et al. 2001), for which energy

Corresponding author address: Andrew S. Kowalski, Departamento de Física Aplicada, Universidad de Granada, Avenida Fuentenueva S/N, 18071 Granada, Spain.
E-mail: andyk@ugr.es

balance closure is a generally unmet validation criterion. To address this deficiency, scientists have dedicated meetings (Foken and Oncley 1995; Foken et al. 2011; Massman and Lee 2002), synthesis analyses (Aubinet et al. 2000; Hendricks Franssen et al. 2010; Moderow et al. 2009; Oncley et al. 2007) and whole projects (Oncley et al. 2007). The lack of closure to date highlights uncertainty in micrometeorological surface exchange estimates (Liu et al. 2006; Twine et al. 2000) and suggests possible errors in basic methodology, within which accurate averaging procedures are critical.

This study demonstrates a tradition of inaccuracy in calculating the averages of important boundary layer state and flow variables, and proposes new rules for atmospheric averaging in general. Section 2 introduces some fundamental mathematical definitions and section 3 combines principles of statistical sampling and physical conservation to show the need to include appropriate weighting functions when determining means for the temperature, mixing ratio, and velocity. The calculation of averages as simple arithmetic means, as is traditional in (micro)meteorology, is shown in section 4 to yield errors in the mean and perturbation variables defining turbulent exchanges. The paper finishes by discussing implications, both in the boundary layer and more globally, of properly determined gas-phase averages for meteorological and climatological purposes, and by presenting general conclusions.

2. Mathematical definitions of averaging

To lay a firm foundation for subsequent analyses, care will be taken to define as precisely as possible a certain mathematical notation that is used frequently in the literature, as well as a new one whose utility is justified beforehand. For applications in modern (micro)meteorology, it is assumed that instruments measure rapidly enough to characterize state and flow variables “at an instant,” despite nonideal instrument responses including the finite time necessary for sonic or electromagnetic waves to traverse a fixed (Eulerian) sensing volume. Given this, we can define x_i as the i th instantaneous realization, representing integration (i.e., an average in some sense) over the sensing volume of the state or flow variable x to which an instrument responds, or other volume such as a model cell. From such “raw data,” meteorological tradition defines the overbar notation where \bar{x} , defined as

$$\bar{x} \equiv \frac{1}{N} \sum_{i=1}^N x_i, \quad (1)$$

denotes the arithmetic mean of N equally weighted samples of x (Galmarini and Thunis 1999). However,

recalling that x_i is itself an average, the fundamentals of statistics do not allow equating \bar{x} with the true mean of x unless every x_i represents a sample population of equal size and therefore deserves equal weight (Bevington and Robinson 2003). This criterion is not generally met by atmospheric data, as is illustrated by the following simple example.

To demonstrate the discrepancy between \bar{x} as defined by Eq. (1) and the true mean of a certain atmospheric variable, let us consider the case of an idealized (e.g., sonic) thermometer whose sensing volume is a cube with 1-mm sides. For elucidatory purposes, we can specify a dry air mixture of standard (constant) atmospheric composition and pressure (1013.25 mb) measured over an arbitrary interval during which the temperature T is -20°C during half the interval, while the remainder of the time it is 20°C . One might assume that the average T over the interval would thus be 0°C , but in fact this would overestimate the true mean considerably, as becomes clear when quantifying air populations via the gas law in the chemist’s form ($PV = nR^*T$; where R^* is the universal gas constant). Since the sensing volume contains more air ($n = 48.1$ nmol) when cold than when warm ($n = 41.6$ nmol), the true mean of T is actually colder than initially supposed. The exact average (nearly 1.5°C below zero) must be calculated via appropriate weighting—in this case according to the amount of dry air present (an extensive quantity) in the sensing volume at each instant—and this leads to a second definition in notation.

Despite the simplification of considering dry air of constant composition, the preceding example demonstrates the need to apply some form of weighting when exactly calculating averages for some atmospheric variables. To describe such weighting, we can define an overwave notation

$$\tilde{x} \equiv \frac{\frac{1}{N} \sum_{i=1}^N a_i x_i}{\frac{1}{N} \sum_{i=1}^N a_i}, \quad (2)$$

where \tilde{x} is the true average of x_i , and a_i is the necessary weighting factor. For the simple (constant composition) example above, the weighting factor for computing the exact mean T is fairly intuitive in a statistical context. Generally, however, when precisely defining the average for any atmospheric state or flow variable, the appropriate weighting factor (if any) must be applied in a manner that is consistent with fundamental conservation principles.

3. Averaging according to physical conservation principles

The atmosphere is governed by laws of conservation of the extensive quantities mass, momentum, and energy (Holton 1992) that must be respected when selecting the appropriate weighting factor to define the averages of state and flow variables. If a population of air samples were mixed together, in an ideal sense with no heating by friction or other physiochemical transformations, then the homogeneous equilibrium state ultimately achieved would correspond to the mean state. For example, a parcel with a premixing T above that of the equilibrium state would be warmer than average and thus capable of heating the rest of the population. The same can be said regarding velocities and trace gas fractions: it is against the final, well-mixed state that we can compare a given parcel to determine its influence on the average. Therefore, in accordance with mixing theory, the means of state and flow variables must be defined by applying conservation principles, sometimes requiring the use of weighting. Consistent with the Eulerian construct describing most instrument sensing volumes (and some model pixels), these conservation principles will be applied here in the context of equal-volume samples.

a. State variables requiring no weighting factor

First we will see how simple arithmetic averaging yields the true mean for certain state variables. The total mass M of N samples with equal volume is simply the sum

$$M = \sum_{i=1}^N m_i, \quad (3)$$

where m_i is the mass of the i th individual. When mixing toward equilibrium, mass conservation dictates that any mass lost by a given subvolume V_i must be gained elsewhere within the population of Eulerian subvolumes under consideration, and so the average mass can be defined exactly as

$$\bar{m} = \frac{1}{N} \sum_{i=1}^N m_i. \quad (4)$$

If each side of Eq. (4) is divided by the sample (e.g., sensing) volume, which is constant ($V_i = V$) and can therefore be moved inside the summation on the right-hand side, then it is readily shown for the state variable known as the density ρ that the average is exactly defined by the arithmetic mean

$$\tilde{\rho} = \bar{\rho} \equiv \frac{1}{N} \sum_{i=1}^N \rho_i. \quad (5)$$

According to this reasoning, for any variable representing the amount of a conserved, extensive quantity per unit of volume, no weighting factor is required ($a_i = 1$) when calculating the average from equal-volume samples.

Recognizing that fluid pressure p is an expression of energy per unit of volume, the energy conservation principle therefore allows us to write directly that the average pressure is

$$\tilde{p} = \bar{p} \equiv \frac{1}{N} \sum_{i=1}^N p_i. \quad (6)$$

However, for other variables we will now see that it is not generally true that $\tilde{x} = \bar{x}$, since conservation laws require the inclusion of different weighting factors for determining their exact averages.

b. State and flow variables requiring a weighting factor

For purposes of specifying sensible heat exchange, it is essential to accurately define the average temperature T of a population of volumes. The conserved, extensive quantity of relevance—in the isobaric context describing atmospheric heating at the surface—is the enthalpy H , a synonym for sensible heat (Petty 2008). Although total enthalpy cannot be measured directly, changes in enthalpy are directly proportional to changes in T , an intensive scalar, when scaled by the product of density ρ and specific heat C_p . In the context of mixing equal-volume samples, this means that the average T of a population is equivalent to the final T of a mixture of air samples with different values of T_i that is allowed to reach equilibrium, and is defined as

$$\tilde{T} \equiv \frac{\frac{1}{N} \sum_{i=1}^N \rho_i C_{p,i} T_i}{\frac{1}{N} \sum_{i=1}^N \rho_i C_{p,i}}, \quad (7)$$

where the weighting factor for Eq. (2) is $a_i = \rho_i C_{p,i}$.

Another intensive scalar of importance in meteorology whose average requires the use of a weighting factor is the mixing ratio, defined as the mass ratio of a constituent (such as CO_2) to dry air [$c \equiv (\rho_c/\rho_d)$]. The mixing and mass conservation concepts expressed above can be applied to both CO_2 and dry air to show that the average mixing ratio is

$$\tilde{c} = \frac{\bar{\rho}_c}{\bar{\rho}_d} = \frac{\frac{1}{N} \sum_{i=1}^N \rho_{c,i}}{\frac{1}{N} \sum_{i=1}^N \rho_{d,i}} = \frac{\frac{1}{N} \sum_{i=1}^N \rho_{d,i} c_i}{\frac{1}{N} \sum_{i=1}^N \rho_{d,i}}, \quad (8)$$

or an average weighted by the dry air density ($a_i = \rho_{d,i}$). Note that Eq. (8) applies to the case of constant-volume (Eulerian) samples and therefore is not valid for measurements made with closed-path gas analyzers that measure at a fixed temperature (Leuning and Judd 1996) and thereby approximate constant mass sampling.

Finally, conservation of momentum (extensive) is the principle to be considered when defining the average velocity (intensive) of any system of particles (such as a fluid), consistent with tradition in classical mechanics. In a constant-volume context, for an arbitrary velocity component u , this takes the form

$$\tilde{u} \equiv \frac{\frac{1}{N} \sum_{i=1}^N \rho_i u_i}{\frac{1}{N} \sum_{i=1}^N \rho_i}, \quad (9)$$

with $a_i = \rho_i$ representing a density-weighted average (Reynolds 1895).

With these definitions for the means \bar{x} of each flow and state variable, we can exactly define perturbation components x'' as

$$x'' \equiv x - \bar{x}, \quad (10)$$

which is an important step toward defining transport by eddies or waves embedded in the mean state and flow.

4. Errors caused by traditional arithmetic averaging

In support of the above definitions, the analyses in this section show that the weighted averages \tilde{T} and \tilde{u} are consistent with the gas law and the definition of the average velocity in classical mechanics, whereas the traditionally employed arithmetic averages \bar{T} and \bar{u} are not. For simplicity, these examinations are restricted to the case of constant (dry) air composition.

a. The gas law and the exact mean temperature

For dry air, the mean temperature defined by Eq. (7) simplifies to a density-weighted average, with greatly simplified notation. The constant specific heat $C_{p,i} = C_p$ can be extracted from the summations in both numerator and denominator of Eq. (7), and so cancels out. When notation defined in Eq. (1) is used this leaves

$$\tilde{T} = \frac{\overline{\rho T}}{\bar{\rho}}, \quad (11)$$

corresponding to the ‘‘Hesselberg averaging’’ operator (Herbert 1995; Kramm 1995; Kramm et al. 1995).

Applying Reynolds’ arithmetic averaging rules to Eq. (11) yields

$$\tilde{T} = \bar{T} + \frac{\overline{\rho' T'}}{\bar{\rho}}. \quad (12)$$

The weighted average temperature \tilde{T} defined in Eqs. (11) and (12) is readily shown to correspond to the mean state of dry air as defined in the gas law. Beginning with the form of the ideal gas law preferred by meteorologists,

$$p = \rho R T \quad (13)$$

(with R representing the gas constant particular to dry air), and following micrometeorological tradition, each state variable can be decomposed into its arithmetic mean \bar{x} and any deviations from therefrom

$$x' \equiv x - \bar{x} \quad (14)$$

to yield

$$\bar{p} + p' = R(\bar{\rho} + \rho')(\bar{T} + T'). \quad (15)$$

Applying Reynolds’ rules of averaging to Eq. (15) leaves

$$\bar{p} = \bar{\rho} R \left(\bar{T} + \frac{\overline{\rho' T'}}{\bar{\rho}} \right), \quad (16)$$

confirming that \bar{T} does not correspond to the true mean air temperature (i.e., that which must be related to \bar{p} and $\bar{\rho}$ via the gas law), and thus that T' is a biased estimate of turbulent perturbations from the mean. By contrast, substituting terms from Eqs. (5), (6), and (7) into Eq. (16) produces

$$\tilde{p} = \tilde{\rho} R \tilde{T}, \quad (17)$$

verifying that the gas law is scale independent when the appropriate temperature \tilde{T} is used to represent the mean, irrespective of the presence of (turbulent-scale) fluctuations whose temperature perturbations should be expressed as T'' , defined by Eq. (10).

b. Classical mechanics and the exact mean velocity

Following a brief review of the traditionally defined mean velocity \bar{u} and its importance and debate in micrometeorology, the validity of \tilde{u} as an exact expression of the mean velocity will be demonstrated using a hypothetical experiment to compare their predicted values versus the definition from classical mechanics. In examining the case of steady-state heat flow in dry air, the

further simplification will be added of considering only the vertical velocity component w . The justification for this lies in the micrometeorological tradition of supposing horizontal homogeneity and focusing on diffusive turbulent transport in the vertical direction, for which gradients and fluxes are of the greatest interest, particularly in the context of surface exchange.

The arithmetic averaging paradigm traditionally has been used, in conjunction with appropriate boundary conditions for the (convective) daytime case, to posit the need for an upward mean airflow to offset a purported downward turbulent flux of dry air associated with density differences between warm updrafts and cool downdrafts. At least as early as half a century ago (Priestley and Swinbank 1947), this offsetting mean flow was derived from the approximation of zero dry air exchange at the surface, and decomposed according to Reynolds' rules as

$$\overline{w\rho} = 0 = \overline{w\rho} + \overline{w'\rho'}. \quad (18)$$

From this, \overline{w} (interpreted incorrectly as the mean vertical wind) was diagnosed and related to the kinematic heat flux density via an approximation of the perturbation ideal gas law as

$$\overline{w} = -\frac{\overline{w'\rho'}}{\overline{\rho}} \approx -\frac{\overline{w'T'}}{\overline{T}}. \quad (19)$$

This diagnosis of a mean flow in the direction of the turbulent heat flux is sometimes termed a “WPL velocity” following the work of Webb et al. (1980), who assessed the relevance of such “density corrections” to scalar (mass) transport. It has furthermore been invoked in the context of advective (Pigeon et al. 2007) or quasi-advective (Massman and Lee 2002; Ono et al. 2008) transport. More recently, however, this supposed mean velocity has been refuted by simple hypsometric analysis and invalidated as not representing a net movement of air (Kowalski and Serrano-Ortiz 2007), a repudiation further supported by the following example.

To illustrate the pitfalls of arithmetic averaging for determining the mean velocity, we can consider the simplest case of a steady-state, convective boundary layer with horizontal homogeneity and null horizontal mean flow. As depicted in Fig. 1, let us stipulate fixed, horizontal boundaries (plates) separated vertically by 100 m, and a superadiabatic lapse rate (unstable case, heated from below and cooled by the upper plate) corresponding to a uniform upward heat flux density of 400 W m^{-2} . This heat exchange is accomplished by turbulence (large Rayleigh number) everywhere in the fluid excepting the thin laminar (molecular) sublayers

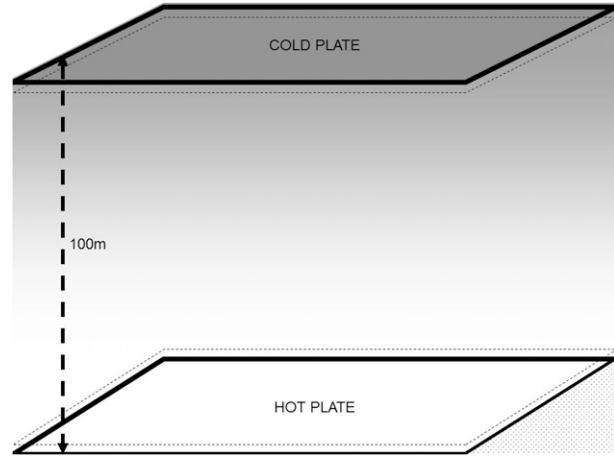


FIG. 1. Depiction of a 100-m-deep turbulent boundary layer separating two horizontal plates, with an upward heat flux density of 400 W m^{-2} .

very near the boundary plates, which we will ignore. Given these parameters, the upward \overline{w} implied by Eq. (19) is everywhere on the order of 1 mm s^{-1} (Webb et al. 1980), an estimate of the mean velocity that is not supported by classical mechanics.

For steady-state conditions, a mean air velocity toward or away from a boundary with null gas exchange is nonsensical. Given the conditions specified above, after 10^5 s (about 27 h) of such steady-state conditions, a 1 mm s^{-1} average velocity would, by its very definition in classical mechanics, imply that the entire fluid be displaced by 100 m (i.e., beyond the upper plate), which is quite absurd. By contrast, the true vertical velocity \tilde{w} defined by the combination of Eq. (9) and the boundary condition expressed in Eq. (18) is exactly zero. Most importantly, the perturbation vertical velocities, determined by subtracting the mean from the fluctuating velocity field and fundamental in the definition of eddy transport, are biased unless \tilde{w} is taken as the true mean.

5. Implications

The preceding analyses insist on the use of weighting to exactly define the means and perturbations of certain atmospheric variables, notwithstanding a long tradition of imprecise averaging practices in (micro)meteorology. The use of inexact arithmetic averaging dates back nearly a century, when density weighting was neglected in reckoning average air velocities over a spatial domain (Taylor 1915). Such practice is often termed Reynolds averaging, despite the fact that Reynolds (1895) unflinchingly defined average velocities via density weighting, in accordance with momentum conservation. Although Reynolds (1895) neglected to decompose ρ , he did so—as

[F1]

his very title makes clear—only when explicitly assuming incompressibility. Such a simplification was valid for his fluid (water), but it is not justified for air. Nonetheless, mainstream micrometeorology—from a midcentury review (Priestley and Sheppard 1952) through standard texts (Foken 2008b; Stull 1988; Sutton 1953) to a twenty-first-century handbook (Moncrieff et al. 2004)—has neglected appropriate weighting and used arithmetic means to define average velocities and temperatures as in Eq. (1) and has thereby erroneously specified turbulent fluctuations. The errors associated with such inexactitude have differing degrees of consequence for estimates of boundary layer transport of mass, versus heat and momentum.

For assessing turbulent mass exchange, boundary layer meteorologists have accurately accounted for “density effects” despite misinterpreting their meanings and erroneously defining the average velocity. This is because the covariance $\overline{w'\rho'_c}$ is only one component of the net transport of a scalar c with density ρ_c , which is accurately expressed by the arithmetic mean $\overline{w\rho_c}$, consistent with momentum conservation (section 3b). No errors arise when decomposing both w and ρ_c into components as in Eq. (14), so long as \bar{w} and w' are not interpreted as representing mean and turbulent components. As has been shown (Webb et al. 1980), the mean constituent flux density

$$\overline{w\rho_c} = \bar{w}\bar{\rho}_c + \overline{w'\rho'_c} \quad (20)$$

is proportional to the covariance between w and the mixing ratio c and can be expressed as $\bar{\rho} \cdot \overline{w'c'}$, describing “diffusive” (advective) transport via the kinematics of a conserved dimensionless proportion (Kowalski and Serrano-Ortiz 2007; Kowalski and Argüeso 2011). The absence of an error in calculating the mean turbulent mass exchange does not, however, apply to the cases of heat and momentum transfer by turbulence.

Unlike mass (but like work), heat is not a quantifiable parcel attribute but purely a transfer variable. Indeed, the calorimetry principle invoked in writing Eq. (7) applies only to substances of different temperatures in thermal contact, consistent with the zeroth law of thermodynamics. Only fluctuations T'' define the possibility of heat exchange: parcels that are relatively warm ($T'' = T - \tilde{T} > 0$) and directed upward ($w'' = w - \tilde{w} > 0$), or those that represent downward ($w'' = w - \tilde{w} < 0$) migration of relatively cold air ($T'' = T - \tilde{T} < 0$), contribute to an upward heat flux; average parcels ($T'' = 0; T = \tilde{T}$) affect no heat transfer, whatever the vertical velocity. The quantity \overline{wT} is not therefore directly related to mean heat transport, nor does it represent the mean of wT , which is not conserved in a

constant volume context. This, plus the fact that traditional fluctuations w' and T' erroneously define heat transport by every eddy, suggests the need to thoroughly revisit turbulent heat transport with averages defined exactly as in section 3b, which may well help close the surface energy budget. Given this disparity between the consequences of inaccurate averaging for the case of mass transport versus heat exchange, corrections to turbulent mass fluxes based on forcing closure of the energy budget (Twine et al. 2000) cannot be justified, although a similar approach might be relevant for characterizing traditional errors in momentum exchange.

As is the case for heat, for momentum transport \overline{wu} cannot be considered as representing the average of wu , which is not conserved in a constant volume context. [Similarly, $\overline{\rho wu}$ is not the exact average of the quantity ρwu , which has been used in an attempt to examine the sensitivity of momentum fluxes to density effects (Fuehrer and Friehe 2002).] The Reynolds stress, traditionally expressed as proportional to $\overline{w'u'}$, derives directly from averaging of the Navier–Stokes equations. Since such averaging traditionally has neglected the physical conservation principles outlined in section 3, both w' and u' represent biased estimates of eddy velocity components, which should rather be calculated from Eqs. (9) and (10). Therefore, momentum transfer as traditionally determined in micrometeorology likely requires correction for density effects and also may merit revisiting in the context of exact averaging procedures.

The tradition of imprecise atmospheric averaging is not limited to micrometeorology and may mean that sizeable errors also have been committed in studies at much larger scales. Fluctuations have been defined against inexact arithmetic averages in studies of transport by mesoscale (Schlesinger 1994) and meridional (Vernekar 1967) eddies, and likely require correction. Experience from micrometeorology suggests that the density corrections implied by adopting exact averaging procedures are far from negligible, at least in the case of mass exchange. Even climatological calculations could be reexamined; the mean air temperature at any given location must be calculated using the appropriate weighting function, or be rendered imprecise. For example, a normal distribution of air temperatures representing equal volume samples that experiences increased variability (i.e., broadens) but no change in the mode (Pachauri et al. 2001) nonetheless necessarily implies net cooling since cold extremes deserve more weight than do hot ones. For the same reason, an exact estimate of the mean global air temperature must result from weighting polar regions more than tropical ones (of equal area and at equal pressure), roughly based on where more air resides but exactly determined by

Eq. (7). The averaging rules arising from these analyses can therefore be considered of global importance in the atmospheric sciences.

6. Conclusions

For temperatures, mixing ratios, and velocities representing constant-volume measurements (or grid cells), exactly determined averages must be specified, not via arithmetic averaging but rather in accordance with physical conservation principles as in Eqs. (7), (8), and (9), respectively. Consequently, eddy velocities determined as deviations from the arithmetic average \bar{w} are in error, as are temperature fluctuations calculated by subtracting the arithmetic average \bar{T} . Mass, heat, and momentum flux densities computed from such perturbation variables are likewise incorrect, except when rectified as via the “density corrections” (Webb et al. 1980) that accurately determine turbulent mass exchange despite incorrectly reckoning average velocities. The importance of such errors on fluxes of heat and momentum remains open to investigation.

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