Air temperature equation derived from sonic temperature and water vapor mixing ratio for turbulent air flow sampled through closed-path eddy-covariance flux systems

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Abstract. Air temperature (T) plays a fundamental role in many aspects of the flux exchanges between the atmosphere and ecosystems. Additionally, it is critical to know where (in relation to other essential measurements) and at what frequency T must be measured to accurately describe such exchanges. In closed-path eddy-covariance (CPEC) flux systems, T can be computed from the sonic temperature (T_s) and water vapor mixing ratio that are measured by the fast-response sensors of a three-dimensional sonic anemometer and infrared gas analyzer, respectively. T is then computed by use of either

\[ T_s + 0.51 \] or

\[ T_s - 0.032 \frac{P}{e} - 1 \]

where q is specific humidity, or \( e \) is water vapor pressure and \( P \) is atmospheric pressure. Converting q and \( e/P \) into the same water vapor mixing ratio analytically reveals the difference between these two equations. This difference in a CPEC system could reach ±0.18 K, bringing an uncertainty into the accuracy of T from both equations and raising the question of which equation is better. To clarify the uncertainty and to answer this question, the derivation of T equations in terms of \( T_s \) and \( H_2O-related \) variables is thoroughly studied. The two equations above were developed with approximations; therefore, neither of their accuracies are evaluated, nor was the question answered. Based on the first principles, this study derives the T equation in terms of \( T_s \) and water vapor molar mixing ratio \( \chi_{H_2O} \) without any assumption and approximation. Thus, this equation itself does not have any inherent error, and the accuracy in T from this equation (equation-computed T) depends solely on the measurement accuracies of \( T_s \) and \( \chi_{H_2O} \). Based on current specifications for \( T_s \) and \( \chi_{H_2O} \) in the CPEC300 series and given their maximized measurement uncertainties, the accuracy in equation-computed T is specified within ±1.01 K. This accuracy uncertainty is propagated mainly (±0.02K) from the uncertainty in \( T_s \) measurements and little (±0.02K) from the uncertainty in \( \chi_{H_2O} \) measurements. Apparently, the improvement in measurement technologies, particularly for \( T_s \) would be a key to narrowing this accuracy range. Under normal sensor and weather conditions, the specified accuracy is overestimated in range and actual accuracy is better. Equation-computed T has a frequency response equivalent to high-frequency \( T_s \) and is insensitive to solar contamination during measurements. As synchronized at a temporal scale of measurement frequency and matched at a spatial scale of measurement volume with all aerodynamic and thermodynamic variables, this T has advanced merits in boundary-layer meteorology and applied meteorology.
1 Introduction

The equation of state, $P = \rho RT$, is a fundamental equation for describing all atmospheric flows where $P$ is atmospheric pressure, $\rho$ is moist air density, $R$ is gas constant for moist air, and $T$ is air temperature (Wallace and Hobbs, 2006). In the boundary-layer flow, where turbulence is nearly always present, accurate representation of the “state” of the atmosphere at any given “point” and time requires consistent representation of spatial and temporal scales for all thermodynamic factors of $P$, $\rho$, and $T$ (Panofsky and Dutton, 1984). Additionally, for observing fluxes describing exchanges of quantities such as heat and moisture between the earth and the atmosphere, it is critical to know all three-dimensional (3-D) components of wind speed at the same location and temporal scale as the thermodynamic variables (Laubach and McNaughton, 1998).

In a closed-path eddy-covariance (CPEC) system, the 3-D wind components and sonic temperature ($T_s$) are measured by a 3-D sonic anemometer in the sonic measurement volume near which air is sampled through the orifice of an infrared gas analyzer (hereafter referred as to infrared analyzer) into its closed-path H2O/CO2 measurement cuvette where air moisture is measured by the analyzer (Fig. 1). The flow pressure inside the cuvette ($P_c$) and the differential ($\Delta P$) between $P_c$ and ambient flow pressure in the sampling location are also measured (Campbell Scientific Inc., 2018c). Atmospheric $P$ in the sampling volume, therefore, is a sum of $P_c$ and $\Delta P$. $P_c$, along with the internal $T$, is further used for infrared measurements of air moisture (i.e., $\rho_w$, H2O density) to calculate the water mixing ratio ($\chi_w$) inside the cuvette that is also equal to $\chi_w$ in the CPEC measurement volume including sonic measurement volume and air sampling location. Finally, the $T_s$ and $\chi_w$ from the CPEC measurement volume, after spatial and temporal synchronization (Horst and Lenschow, 2009), are used to calculate the $T$ inside this volume. Two optional equations (Schotanus et al., 1983; Kaimal and Gaynor, 1991; see the section of Background), which need rigorous evaluation, are available for this $T$ calculation. In summary, the boundary-layer flow measured by a CPEC system has all variables quantified with consistent representation of spatial and temporal scales for moist turbulence thermodynamics (i.e., state) if the following are available: 3-D wind, $P$ measured differentially; $T$ from an equation; and $\rho$ from $P$, $T$, and $\chi_w$. 
In this paper, we derive a $T$ equation in terms of $T_s$ and $\chi_w$ based on the first principles as an alternative to the commonly used equations that are based on approximations; 2) estimate and verify the accuracy of the first-principles $T$; 3) assess the expected advantages of the first-principles $T$ as a high-frequency signal insensitive to solar contamination suffered by conventional $T$ sensor measurements (Lin et al., 2001; Blonquist and Bugbee, 2018); and 4) briefly address the potential applications of the derived $T$ equation in flux measurements. We first provide a brief summary of the moist turbulence thermodynamics of the boundary-layer flows measured by CPEC flux systems.

2 Background

A CPEC system is commonly used to measure boundary-layer flows for the CO$_2$, H$_2$O, heat, and momentum fluxes between ecosystems and the atmosphere. Such a system is equipped with a 3-D sonic anemometer to measure the speed of sound in three dimensions in the central open-space of the instrument (hereafter referred to as open-space), from which can be calculated $T$, $T_s$, and 3-D components of wind at fast response. Integrated with this sonic anemometer, a fast-response infrared gas analyzer concurrently measures CO$_2$ and H$_2$O in its cuvette (closed-space) of infrared measurements, through which air is sampled under pump pressure while being heated (Fig. 1). The analyzer outputs the CO$_2$ mixing ratio (i.e., $\chi_{CO_2} = \rho_{CO_2}/\rho_d$, where $\rho_{CO_2}$ is CO$_2$ density and $\rho_d$ is dry air density) and $\chi_w$ (i.e., $\rho_w/\rho_d$). Together, these instruments provide high-frequency (e.g., 10 Hz) measurements from which the fluxes are computed (Aubinet et al., 2012) at a “point” represented by the sampling space of the CPEC system.

These basic high-frequency measurements of 3-D wind speed, $T_s$, $\chi_w$, and $\chi_{CO_2}$ provide observations from which mean and fluctuation properties of air, such as $\rho$, $\rho_d$, $\rho_{CO_2}$, and $\chi_w$, fluxes can be determined. For instance, water vapor flux is
calculated from \( \rho_d \chi_w \), where \( v \) is vertical velocity of air and prime indicates the fluctuation of variable away from its mean as indicated by overbar (e.g., \( \bar{w} = w - \bar{w} \)). Given the measurements of \( \chi_w \) and \( P \) from CPEC systems, \( \rho_d \) is derived from

\[
\rho_d = \frac{P}{T(R_o + R_v,)}
\]  

(1)

where \( R_o \) is gas constant for dry air and \( R_v \) is gas constant for water vapor. In turn, \( \rho_d \) is equal to \( \rho_d \chi_w \) and \( \rho \) is a sum of \( \rho_d \) and \( \rho_v \). All mentioned physical properties can be derived if \( T \) in Eq. (1) is acquired.

Additionally, equations for ecosystem exchange and flux require \( \bar{\rho}_d \) (Gu et al., 2012) and \( \bar{\rho}_d \chi_w \) (Foken et al., 2012). Furthermore, due to accuracy limitations in measurements of \( w \) from a modern sonic anemometer, the dry air flux of \( \rho_d \) must be derived from \( \bar{\rho}_d \chi_w \) - \( \bar{\rho}_d \chi_w \) (Webb et al., 1980; Lee and Massman, 2011). Because of its role in flux measurements, a high-frequency representation of \( \rho_d \) is needed. To acquire such \( \rho_d \) from Eq. 1 for advanced applications, high-frequency \( T \) in temporal synchronization with \( \chi_w \) and \( P \) is needed.

In a modern CPEC system, \( P \) is measured using a fast-response barometer suitable for measurements at a high frequency (e.g., 10 Hz, Campbell Scientific Inc., 2018a) and, as discussed above, \( \chi_w \) is a high-frequency signal from a fast-response gas analyzer (e.g., commonly up to 20 Hz). If \( T \) is measured using a slow-response sensor, the three independent variables in Eq. (1) do not have equivalent synchronicity in frequency response. In terms of frequency response, \( \rho_d \) cannot be correctly acquired. \( \rho_d \) derived based on Eq. 1 also has uncertainty, although it can be approximated from either of the following equations:

\[
\bar{\rho}_d = \frac{P}{T(R_o + R_v,)}
\]  

(2)

and

\[
\bar{\rho}_d = \frac{P}{T(R_o + R_v,)}
\]  

(3)

Eq. (2) is mathematically valid in averaging rules (Stull, 1988), but the response of the system to \( T \) is slower than to \( \chi_w \) and even \( P \), while the Eq. (3) is invalid under averaging rules although its three over-bar independent variables can be evaluated over an average interval. Consequently, neither \( \rho_d \chi_w \) nor \( \bar{\rho}_d \chi_w \) can be evaluated strictly in theory.

Measurements of \( T \) at high frequency (similar to those at low-frequency) are contaminated by solar radiation, even under shields (Lin et al., 2001) and when aspirated (Campbell Scientific Inc., 2010; R.M. Young Company, 2004; Apogee Instrument Inc., 2013; Blonquist and Bugbee, 2018). Additionally, the aspiration method cannot acquire \( T \) at high frequency due to the disturbance of an aspiration-fan to natural turbulent flows, and fine wires and aspiration methods have limited applicability for long-term measurements in rugged field conditions typically encountered in ecosystem monitoring.

To avoid the issues above in use of either slow- or fast-response \( T \) sensors under field conditions, deriving \( T \) from \( T_s \) and \( \chi_w \) (Schotanus et al., 1983; Kaimal and Gaynor, 1991) is an advantageous alternative to the applications of \( T \) in CPEC measurements and is a significant technology for instrumentation to pursue. In a CPEC system, \( T \) is measured at a high frequency (e.g., 10 Hz) using a fast-response sonic anemometer to detect the speed of sound in the open-space (Munger et al.,
provided there is no evidence of contamination by solar radiation. It is a high-frequency signal. \( \chi_w \) is measured at the same frequency as for \( T_s \) using a gas analyzer equivalent to the sonic anemometer in high-frequency response time (Ma et al., 2017). \( \chi_w \) reported from a CPEC system is converted from water vapor molar density measured inside the closed-space cuvette whose internal pressure and internal temperature are more stable than \( P \) and \( T \) in the open-space and can be more accurately measured. Because of this, solar warming and radiation cooling of the cuvette is irrelevant, as long as water molar density, pressure, and temperature inside the closed-space cuvette are more accurately measured. Therefore, it could be reasonably expected that \( T \) calculated from \( T_s \) and \( \chi_w \) in a CPEC system should be a high-frequency signal insensitive to solar radiation.

The first of two equations commonly used to compute \( T \) from \( T_s \) and air moisture-related variables given by Schotanus et al. (1983) is:

\[
T = T_s [1 + 0.51 \frac{q}{\rho} ]^{-1},
\]  

(4)

where \( q \) is specific humidity, defined as a ratio of water vapor to moist air density. The second equation is given by Kaimal and Gaynor (1991), as:

\[
T = T_s \left[ 1 + 0.32 \frac{R T \rho_0}{R T \rho + R T \rho_0} \right]^{-1} = T_s \left[ 1 + 0.51 \frac{\chi_w}{1 + 161 \chi_w} \right]^{-1}.
\]  

(5)

where \( e \) is water vapor pressure. Re-arranging these two equations gives \( T \) in terms of \( T_s \) and \( \chi_w \). Expressing \( q \) in terms of \( \rho_d \) and \( \rho_w \), Eq. (4) becomes

\[
T = T_s \left[ 1 + 0.51 \frac{\rho_d}{\rho_d + \rho_w} \right]^{-1} = T_s \left[ 1 + 0.51 \frac{\chi_w}{1 + 161 \chi_w} \right]^{-1},
\]  

(6)

and expressing \( e \) and \( P \) using the equation of state, Eq. (5) becomes

\[
T = T_s \left[ 1 + 0.32 \frac{R T \rho_0}{R T \rho + R T \rho_0} \right]^{-1} = T_s \left[ 1 + 0.51 \frac{\chi_w}{1 + 161 \chi_w} \right]^{-1}.
\]  

(7)

The \( \chi_w \)-related terms in the denominator inside parentheses in both equations above clearly reveal that \( T \) values from the same \( T_s \) and \( \chi_w \) using the two commonly used Eqs. (4) and (5) will not be the same. The absolute difference in the values \( \Delta T_e \), i.e., the difference in \( T \) between Eqs. (4) and (5), can be analytically expressed as:

\[
\Delta T = \frac{0.31 T \chi_w^2}{1 + 3.63 \chi_w + 3.20 \chi_w^2}.
\]  

(8)

Given that, in a CPEC system, the sonic anemometer has an operational range in \( T_s \) of -30 to 57 °C (Campbell Scientific Inc., 2018b) and a gas analyzer has a measurement range in \( \chi_w \) of 0 to 0.045 kgH\(_2\)O kg\(^{-1}\) (Campbell Scientific Inc., 2018a), \( \Delta T_e \) ranges up to 0.177 K, which brings an uncertainty in accuracy of \( T \) calculated from either Eq. (4) or (5) and raises the question of which equation is better.

Reviewing the sources of Eq. (4) (Schotanus et al., 1983; Swiatek, 2009; van Dijk, 2002) and Eq. (5) (Ishii, 1932; Barrett and Suomi, 1949; Kaimal and Businger, 1963; Kaimal and Gaynor, 1991), it was found that approximation procedures were used in derivation of both equations, but the approach to the derivation of Eq. (4) (Appendix A) is different from that of Eq. (5) (Appendix B). These different approaches create a difference in disparity between the two commonly used equations as shown in Eq. (8), and the approximation procedures lead to the controversy as to which equation is more accurate. The controversy can be avoided if the \( T \) equation in terms of \( T_s \) and \( \chi_w \) can be derived from the \( T_s \) equation and the first-principles equations, if possible,
without an approximation and verified against precision measurements of \( T \) with minimized solar contamination.

### 3 Theory Derivation of air-temperature equation

As discussed above, a sonic anemometer measures the speed of sound \( (c) \) concurrently with measurement of the 3-D wind speed (Munger et al., 2012). The speed of sound in the homogeneous atmospheric boundary-layer is defined by Barrett and Suomi (1949) as:

\[ c^2 = \frac{\gamma P}{\rho}, \]  

(9)

where \( \gamma \) is the ratio of moist air specific heat at constant pressure \((C_p)\) to moist air specific heat at constant volume \((C_v)\).

Substitution of the equation of state into Eq. (9), gives \( T \) as a function of \( c \):

\[ T = \frac{c^2}{\gamma R}. \]  

(10)

This equation reveals the opportunity to use measured \( c \) for the \( T \) calculation; however, both \( \gamma \) and \( R \) depend on air humidity, which is unmeasurable by a sonic anemometry itself; Eq. (10) is, therefore, not applicable for \( T \) calculations inside a sonic anemometer. Alternatively, \( \gamma \) is replaced with its counterpart for dry air \( [\gamma_d, 1.4003] \), i.e., the ratio of dry air specific heat at constant pressure \((C_{pd})\) to dry air specific heat at constant volume \((C_{vd})\) and \( R \) is replaced with its counterpart for dry air \((R_d, 287.06 \text{ J K}^{-1} \text{ kg}^{-1})\), i.e., gas constant for dry air). Both replacements make the right side of Eq. (10) become \( c^2\gamma_d R_d \) which is no longer a measure of \( T \). However, \( \gamma_d \) and \( R_d \) are close to their respective values of \( \gamma \) and \( R \) in magnitude, and, after the replacements, the right side of Eq. (10) after the replacements is defined as sonic temperature \((T_s)\), given by (Campbell Scientific Inc., 2018b):

\[ T_s = \frac{c^2}{\gamma_d R_d}. \]  

(11)

Comparing this equation to Eq. (10), given \( c \), if air is dry, \( T \) must be equal to \( T_s \); therefore, the authors define **sonic temperature of moist air is the temperature that its dry air component reaches when moist air has the same enthalpy**. Since both \( \gamma_d \) and \( R_d \) are constants and \( c \) is measured by a sonic anemometer and corrected for crosswind effect inside the sonic anemometer based on its 3-D wind measurements (Liu et al., 2001; Zhou et al., 2018), Eq. (11) is used inside the operating system of modern sonic anemometers to report \( T_s \) instead of \( T \).

Equations (9) to (11) provide a theoretical basis of first principles to derive the relationship of \( T \) to \( T_s \) and \( \chi_w \). In Eq. (9), \( \gamma \) and \( \rho \) vary with air humidity and \( P \) is related to \( \rho \) as described by the equation of state. Consequently, the derivation of \( T \) from \( T_s \) and \( \chi_w \) for CPEC systems needs to address the relationship of \( \gamma, \rho, \chi_w \) to air humidity in terms of \( \chi_w \).

#### 3.1 Relationship of \( \gamma \) to \( \chi_w \)

For moist air, the ratio of specific heat at constant pressure to specific heat at constant volume is:

\[ \gamma = \frac{C_p}{C_v}, \]  

(12)

where \( C_p \) varies with air moisture between \( C_{pw} \) and \( C_{pd} \) (water vapor specific heat at constant pressure, 1,952 J kg\(^{-1}\) K\(^{-1}\)). It is the arithmetical average of \( C_{pw} \) and \( C_{pd} \) weighted by dry air mass and water vapor mass, respectively, given by (Stull, 1988; Swiatek,
(2009):

\[ C_p = \frac{C_{pd} P_d + C_{pw} P_w}{\rho_d + \rho_w} \]  

(13)

Based on the same rationale, \( C_v \) is:

\[ C_v = \frac{C_{vd} P_d + C_{vw} P_w}{\rho_d + \rho_w} \]  

(14)

where \( C_{vw} \) is the specific heat of water vapor at constant volume (1,463 J kg\(^{-1}\) K\(^{-1}\)). Substituting Eqs. (13) and (14) into Eq. (12) generates:

\[ \gamma = \frac{1 + \left(\frac{C_{vw}}{C_{pd}}\right) \chi_w}{1 + \left(\frac{C_{vw}}{C_{pd}}\right) \chi_v} \]  

(15)

### 3.2 Relationship of \( P/\rho \) to \( \chi \)

Atmospheric \( P \) is the sum of \( P_d \) and \( e \). Similarly, \( \rho \) is the sum of \( \rho_d \) and \( \rho_w \). Using the equation of state, the ratio of \( P \) to \( \rho \) can be expressed as:

\[ \frac{P}{\rho} = \frac{R_d P_d + R_w P_w}{\rho_d + \rho_w} = \frac{R_d T \left(1 + \frac{R_w}{R_d} \chi_w\right)}{1 + \chi_w} \]  

(16)

In this equation, the ratio of \( R \), to \( R_d \) is given by:

\[ \frac{R}{R_d} = \frac{R^* / M_w}{R / M_d} = \frac{1}{M_w / M_d} \]  

(17)

where \( R^* \) is the universal gas constant, \( M_w \) is the molecular mass of water vapor (18.0153 kg kmol\(^{-1}\)), and \( M_d \) is the molecular mass of dry air (28.9645 kg kmol\(^{-1}\)). The ratio of \( M_w \) to \( M_d \) is 0.622, conventionally denoted by \( \varepsilon \). Substituting Eq. (17), after its denominator is represented by \( \varepsilon \), into Eq. (16) leads to:

\[ \frac{P}{\rho} = \frac{R_d T (\varepsilon + \chi_w)}{\varepsilon (1 + \chi_w)} \]  

(18)

### 3.3 Relationship of \( T_s \) to \( T \) and \( \chi \)

Substituting Eqs. (15) and (18) into Eq. (9), \( c^2 \) is expressed in terms of \( T \) and \( \chi \) along with atmospheric physics constants.

Further, substituting \( c^2 \) into Eq. (11) generates:

\[ c^2 = \frac{R_d \gamma_T (\varepsilon + \chi_w) \left[1 + \left(\frac{C_{pw}}{C_{pd}}\right) \chi_w\right]}{\varepsilon (1 + \chi_w) \left[1 + \left(\frac{C_{pw}}{C_{pd}}\right) \chi_w\right]} \]  

(19)

Further, substituting \( c^2 \) into Eq. (11) generates:

\[ T_s = \frac{T (\varepsilon + \chi_w) \left[1 + \left(\frac{C_{pw}}{C_{pd}}\right) \chi_w\right]}{\varepsilon (1 + \chi_w) \left[1 + \left(\frac{C_{pw}}{C_{pd}}\right) \chi_w\right]} \]  

(20)

Note: This equation (20) now expresses \( T_s \) in terms of \( T \) of interest to this study, \( \chi \), measured in CPEC systems, and atmospheric...
physics constants (i.e., \(\varepsilon\), \(C_{pw}\), \(C_{pd}\), \(C_{vw}\), and \(C_{vd}\)).

### 3.4 Air temperature equation

Rearranging the terms in Eq. (20) results in

\[
T = T_s \left[ \frac{\left( 1 + \varepsilon \right) \left( 1 + \left( C_{vw} / C_d \right) \chi_w \right)}{\left( 1 + \varepsilon \right) \left( 1 + \left( C_{vd} / C_d \right) \chi_d \right)} \right]^{\gamma_v}
\]

(21)

This equation shows that \(T\) is a function of \(T_s\) and \(\chi\) that are measured at high frequency in a CPEC system by a sonic anemometer and an infrared analyzer.

A CPEC system outputs water vapor molar mixing ratio (Campbell Scientific Inc., 2018a) commonly used in the community of eddy-covariance fluxes (AmeriFlux, 2018). The relation of water vapor mass to molar mixing ratio (\(\chi_{H_2O}\) in mol\(H_2O\) mol\(^{-1}\)) is given by:

\[
\chi_{H_2O} = \frac{M_{H_2O}}{M_\chi} \chi_{H_2O} = \chi_{H_2O}.
\]

(22)

Substituting this relation into Eq. (21) and denoting \(C_{vw} / C_{vd}\) with \(\gamma_v = 2.04045\) and \(C_{pd} / C_{pw}\) with \(\gamma_p = 1.94422\), Eq. (21) is expressed as:

\[
T = T_s \left[ \frac{\left( 1 + \varepsilon \right) \chi_{H_2O} \left( 1 + \varepsilon \gamma_v \chi_{H_2O} \right)}{\left( 1 + \varepsilon \right) \chi_{H_2O} \left( 1 + \varepsilon \gamma_p \chi_{H_2O} \right)} \right]^{\gamma_v}
\]

(23)

This is the air temperature equation in terms of \(T_s\) and \(\chi_{H_2O}\) for use in CPEC systems. It is derived from a theoretical basis of first principles [i.e., Eqs. (9) to (11)]. In its derivation, except for the use of the equation of state and Dalton’s law, no other assumptions nor approximations are used. Therefore, Eq. (23) is an exact equation of \(T\) in terms of \(T_s\) and \(\chi_{H_2O}\) for the turbulent air flow sampled through a CPEC system and thus avoids the controversy in use of Eqs. (4) and (5) arising from approximations as shown in Appendices A and B. Therefore, \(T\) computed from this equation (hereinafter referred to as equation-computed \(T\)) should be accurate as long as the values of \(T_s\) and \(\chi_{H_2O}\) are exact.

For this study, however, \(T_s\) and \(\chi_{H_2O}\) are measured by the CPEC systems deployed in the field under changing weather conditions through four seasons. Their measured values must include measurement uncertainty in \(T_s\), denoted by \(\Delta T_s\), and in \(\chi_{H_2O}\) as well, denoted by \(\Delta \chi_{H_2O}\). The uncertainties, \(\Delta T\) and/or \(\Delta \chi_{H_2O}\), unavoidably propagate to create uncertainty in equation-computed \(T\), denoted by \(\Delta T\), which makes an exact \(T\) impossible. In numerical analysis (Burden and Faires, 1993) or in statistics (Snedecor and Cochran, 1991), any applicable equation requires the specification of an uncertainty term. Therefore, the equations for \(T\) should include specification of their respective uncertainty expressed as the bounds (i.e., the maximum and minimum limits) specifying the range of the equation-computed \(T\) that need to be known for any application. According to the definition of accuracy that was advanced by the International Organization for Standardization (2012), this uncertainty range is equivalent to the “accuracy” and the range contributed by both systematic errors (trueness) and random variability (precision). Apparently, \(\Delta T_s\) is the accuracy of \(T_s\) measurements and \(\Delta \chi_{H_2O}\) is the accuracy of \(\chi_{H_2O}\) measurements. Both should be evaluated from their measurement uncertainties, respectively. The accuracy of equation-computed \(T\) is \(\Delta T\). It should be specified through its relationship to \(\Delta T_s\) and \(\Delta \chi_{H_2O}\).
3.5 Relationship of $\Delta T$ to $\Delta T_s$ and $\Delta \chi_{SO_2}$

As measurement accuracies, $\Delta T$ and $\Delta \chi_{SO_2}$ can be reasonably considered as small increments in a calculus sense. As such, depending on both small increments, $\Delta T$ is the total differential of $T$ with respect to $T_s$ and $\chi_{SO_2}$ given by:

$$\Delta T = \frac{\partial T}{\partial T_s} \Delta T_s + \frac{\partial T}{\partial \chi_{SO_2}} \Delta \chi_{SO_2}$$

(24)

The two partial derivatives in the right side of this equation can be derived from Eq. (23). Substituting the two partial derivatives into this equation leads to

$$\Delta T = \frac{T}{T_s} \Delta T_s + \left[ \frac{\epsilon + \epsilon_f (1 + 2 \chi_{SO_2})}{1 + \chi_{SO_2}} \right] \Delta \chi_{SO_2}$$

(25)

This equation indicates that in dry air when $T = T_s$, $\Delta T$ is equal to $\Delta T_s$ if $\chi_{SO_2}$ is measured accurately (i.e., $\Delta \chi_{SO_2} = 0$ while $\chi_{SO_2} = 0$). However, air in the atmospheric boundary-layer where CPEC systems are used is always moist. Given this equation, $\Delta T$ at $T_s$ and $\chi_{SO_2}$ can be evaluated by using $\Delta T_s$ and $\Delta \chi_{SO_2}$, both of which are related to the measurement specifications of sonic anemometers for $T_s$ (Campbell Scientific Inc., 2018b) and of infrared analyzers for $\chi_{SO_2}$ (Campbell Scientific Inc., 2018a). Sonic anemometers and infrared analyzers with different models and brands have different specifications from their manufacturers. Any combination of sonic and infrared instruments has a combination of the $\Delta T_s$ and $\Delta \chi_{SO_2}$ that are specified by their manufacturers. In turn, from Eq. (25), the combination generates $\Delta T$ of equation-computed $T$ for the corresponding combination of the sonic and infrared instruments with given models and brands. Therefore, Eqs. (23) and (25) are applicable to any CPEC system beyond our study brand.

In the right side of Eq. (25), the first term with $\Delta T_s$ can be expressed as $\Delta T_{\epsilon_s}$ (i.e., uncertainty portion of $\Delta T$ due to $\Delta T_s$) and the second term with $\Delta \chi_{SO_2}$ can be expressed as $\Delta T_{\epsilon_{\chi_{SO_2}}}$ (i.e., uncertainty portion of $\Delta T$ due to $\Delta \chi_{SO_2}$). Using $\Delta T_{\epsilon_s}$ and $\Delta T_{\epsilon_{\chi_{SO_2}}}$, this equation can be simplified as:

$$\Delta T = \Delta T_{\epsilon_s} + \Delta T_{\epsilon_{\chi_{SO_2}}}$$

(26)

Assessment on the accuracy of equation-computed $T$ is to evaluate $\Delta T_{\epsilon_s}$ and $\Delta T_{\epsilon_{\chi_{SO_2}}}$ correspondingly from $\Delta T_s$ and $\Delta \chi_{SO_2}$.

4. Accuracy of equation-computed $T$

The CPEC system for this study is CPEC310 (Campbell Scientific Inc., Logan, UT, USA), including whose major components are a CSAT3A sonic anemometer (updated version in 2016) for fast response to 3-D wind and $T_s$ and an EC155 infrared analyzer for fast response to H$_2$O along with CO$_2$ (Burgon et al., 2015; Ma et al., 2017). The system operates in a $T$ range of -30 to 50 °C and measures $\chi_{SO_2}$ in a range up to 79 mmol H$_2$O mol$^{-1}$ (i.e., 37 °C dew point temperature at 86 kPa under manufacturer environment); therefore, the accuracy of equation-computed $T$, depending on $\Delta T_s$ and $\Delta \chi_{SO_2}$, should be defined and estimated in a domain over both ranges.

4.1 $\Delta T_s$ (measurement accuracy in $T_s$)

As is true for other sonic anemometers (e.g., Gill Instruments, 2004), the CSAT3A has not been assigned a $T_s$ measurement performance (Campbell Scientific Inc., 2018b) because the theories and methodologies of how to specify this performance, to the
best of our knowledge, have not been clearly defined. The performance of the CSAT series for \( T \) is best near production temperature around 20 °C and drifts little away from this temperature. Within the operational range of a CPEC system in ambient air temperature, the updated version of CSAT3A has an overall uncertainty to be ±1.00 °C (i.e., \( |ΔT| < 1.0 \text{ K} \))

4.2 \( ΔT_{\text{unc}} \) (Uncertainty in \( H_2O \) measurement)

The accuracy in \( H_2O \) measurements from infrared analyzers, depending upon, depends primarily on analyzer measurement performance. This performance is specified using four component uncertainties: (1) precision variability (\( σ_{\text{un}} \)), (2) maximum zero drift range with ambient air temperature (\( ΔT_{\text{zer}} \)), (3) maximum gain drift with ambient air temperature (\( ΔT_{\text{g}} \)), and (4) cross-sensitivity to \( CO_2 \) (LI-COR Bioscience, 2016; Campbell Scientific Inc., 2018c). Zhou et al. (2021) composited the four component uncertainties as an accuracy model formulated as the \( H_2O \) accuracy equation for CPEC systems applied in ecosystems, given by:

\[
ΔX_{H_2O} = 2 \left[ 196σ_{H_2O} + 585k_0 \right] \left[ \frac{V_{\text{ref}}}{T_a-T_r} + \delta_{H_2O} \epsilon X_{H_2O} \right] \times \left[ \begin{array}{c} T_r > T > T_h \ 
T_r > T > T_s \ 
T_r > T > T_l \ 
T_r > T > T_{rl} \ 
\end{array} \right] - \left[ \begin{array}{c} T_r < T < T_h \ 
T_r < T < T_s \ 
T_r < T < T_l \ 
T_r < T < T_{rl} \ 
\end{array} \right].
\]  

(27)

where \( T_r \) is ambient air temperature at which an infrared analyzer was calibrated by the manufacturer to fit its working equation or zeroed/spanned in the field to adjust the zero/gain drift; subscripts rh and rl indicate the range highest and range lowest values, respectively, and \( T_{rl} \) and \( T_{rl} \) are the highest- and the lowest- \( T \) respectively, over the operational range of CPEC systems in \( T \).

Given the infrared analyzer specifications: \( σ_{H_2O} \), \( k_0 \), \( δ_{H_2O} \), \( T_{rl} \) and \( T_{rl} \), this equation can be used to estimate \( ΔX_{H_2O} \) in Eq. (25) and eventually for \( ΔT_{\text{unc}} \). In (Eq. 26) over the domain of \( T \) and \( X_{H_2O} \).

4.3 \( ΔT \) (Accuracy of equation-computed \( T \))

The accuracy of equation-computed \( T \) can be evaluated using \( ΔT \) and \( ΔX_{H_2O} \) (Eq. 25), varying with \( T \), \( T_a \) and \( X_{H_2O} \). Both \( T \) and \( T_a \) reflect air temperature, being associated with each other through \( X_{H_2O} \) (Eq. 23). Given \( X_{H_2O} \), \( T \) can be calculated from \( T_a \) and vice versa; therefore, for the figure presentations in this study, it is sufficient to use either \( T \) or \( T_a \), instead of both, to show \( ΔT \) with air temperature. Considering \( T \) to be of interest to this study, \( T \) will should be used as such. \( ΔT \) can be analyzed over a domain of \( T \) and \( X_{H_2O} \) within the operational range of CPEC systems in \( T \) from -30 to 50 °C across the analyzer measurement range of \( X_{H_2O} \) from 0 to 0.079 molH\(_2O\) mol\(^{-1}\).

To visualize the relationship of \( ΔT \) with \( T \) and \( X_{H_2O} \), \( ΔT \) is presented better as ordinate along with \( T \) as abscissa associated with \( X_{H_2O} \).

However, due to the positive dependence of air water vapor saturation on \( T \) (Wallace and Hobbs, 2006), \( X_{H_2O} \) has a possible range wider at higher \( T \) and narrower at lower \( T \). To present \( ΔT \) over the same measure of air moisture even at different \( T \), the saturation water vapor pressure is used to scale air moisture to 0, 20, 40, 60, 80 and 100 (i.e., RH, relative humidity in %). For each scaled RH value, \( X_{H_2O} \) can be calculated at different \( T \) and \( P \) (Appendix C) for use in Eq. (25). In this way, over the range of \( T \), the trend of \( ΔT \) due to each measurement uncertainty source can be shown along the curves with equal RH as the measure of air moisture (Fig. 2).
Figure 2: Accuracy of air temperature computed from Eq. (23) (equation-computed $T$) over the measurement range of $\text{H}_2\text{O}$ molar mixing ratio ($\chi_{\text{H}_2\text{O}}$) within the operational range of $T$ for CPEC300 series (Campbell Scientific Inc., UT, USA). a. Accuracy component of equation-computed $T$ due to sonic temperature ($T_s$) measurement uncertainty, b. Accuracy component of equation-computed $T$ due to $\chi_{\text{H}_2\text{O}}$ molar mixing ratio measurement uncertainty, and c. Overall accuracy of equation-computed $T$. 
4.3.1 $\Delta T_s$ (Uncertainty portion of $\Delta T$ due to $T_s$)

Given $\Delta T_s = \pm 1.00$ K and $T_s$ from the algorithm in Appendix C, $\Delta T_s$ in Eq. (26) was calculated over the domain of $T$ and $\chi_{ao}$ (Fig. 2a). Over the whole $T$ range, the $\Delta T_s$ limits range $\pm 1.00$ K, becoming a little narrower with $\chi_{ao}$ increasing due to decrease, at the same $T_s$. In the magnitude $T/T_s$ in Eq. (25). The narrowest limits of $\Delta T_s$, in an absolute value, varies $< 0.01$ K over the range of $T$ below 20 °C although $> 0.01$ K but $< 0.03$ K above 20 °C but $< 0.03$ K.

4.3.2 $\Delta T_{x_{ao}}$ (Uncertainty portion of $\Delta T$ due to $\Delta x_{ao}$)

Given $\chi_{ao}$ from the algorithm in Appendix C and $\Delta x_{ao}$ from Eq. (27), $\Delta T_{x_{ao}}$ was calculated over the domain of $T$ and $\chi_{ao}$ (Fig. 2b). The parameters in Eq. (27) are given through the specifications of the CPEC300 series (Campbell Scientific Inc., 2018a, 2018c). $\sigma_{ao}$ is $6.0 \times 10^{-6}$ mol H$_2$O mol$^{-1}$ where mol is a unit for dry air; $d_{ao}$, $\pm 5 \times 10^{-5}$ mol H$_2$O mol$^{-1}$ with $T$, $\delta_{ao,T}$, 0.30% with $T$; $x_c$, $\pm 5 \times 10^{-8}$ mol H$_2$O mol$^{-1}$ (mmol CO$_2$ mol$^{-1}$); $T_s$, 20 °C as Normal Temperature (Wright et al., 2003); $T_{ao}$, -30 °C, and $T_{ao}$, 50 °C.

As shown in Fig. 2b, $\Delta T_{x_{ao}}$ tends to be smallest at $T = T_s$. However, away from $T_s$, its range non-linearly becomes wider, very gradually widening below $T_s$ but widening more abruptly above, because, as temperature increases, $\chi_{ao}$ at the same RH increases exponentially (Eqs. (c1) and (c5) in Appendix C) while $\Delta x_{ao}$ increases linearly with $\chi_{ao}$ in Eq. (27). This non-linear range can be summarized to be $\pm 0.01$ K below 30 °C and $\pm 0.02$ K above 30 °C. Compared to $\Delta T_s$, $\Delta T_{x_{ao}}$ is much smaller at two orders. $\Delta T_{x_{ao}}$ is a large component in $\Delta T$.

4.3.3 $\Delta T$ (Combined uncertainty as the accuracy in equation-computed $T$)

Equation (26) is used to determine the maximum combined uncertainty in equation-computed $T$ for the same RH grade in Fig. 2 by adding together the same sign (i.e., $+$) curve data of $\Delta T_s$ in panel Fig. 2a and $\Delta T_{x_{ao}}$ in panel Fig. 2b. $\Delta T$ ranges at different RH grades are shown in panel Fig. 2c. This panel Figure 2c can specify the accuracy of equation-computed $T$ at 101.325 kPa [i.e., Normal Atmospheric Pressure as used by Wright et al. (2003)] over the $\chi_{ao}$ measurement range to be within $\pm 0.02$ K. This accuracy for high-frequency $T$ currently is the best in turbulent flux measurement because $\pm 0.00$ K is the best in accuracy of $T_s$ from the individual sonic anemometers which are widely used for sensible heat flux in almost all CPEC systems.

4.4 Accuracy of equation-computed $T$ from CPEC field measurements

Equation (23) is derived particularly for CPEC systems in which $T_s$ and $\chi_{ao}$ are measured neither at the same volume nor at the same time. Both variables are measured separately using a sonic anemometer and an infrared analyzer in a spatial separation between the $T_s$ measurement center and the $\chi_{ao}$ measurement cuvette (e.g., Fig. 1), along with a temporal lag in the measurement of $\chi_{ao}$ relative to $T_s$ due to the transport time and phase shift (Ibrom et al., 2007) of turbulent air flows sampled for $\chi_{ao}$ through the sampling orifice to the measurement cuvette (Fig. 3).
Fortunately, the spatial separation scale is at the tens of centimeters scale and the temporal lag scale is of the tens of milliseconds scale. In eddy-covariance flux measurements, such a separation misses some covariance signals at higher frequency, which is correctable (Moore, 1986), and such a lag diminishes the covariance correlation, which is recoverable (Ibrom et al., 2007). How such a separation along with the lag influences the accuracy of Eq. (23), as shown in Fig. 2, needs testing against precision measurements of air temperature. The two advantages of the equation-computed $T$ discussed in the introduction, namely the fast response to high frequency signals and the insensitivity to solar contamination in measurements, were studied and assessed during testing when a CPEC system was set up in the Campbell Scientific Instrument Test Field (41.8°N, 111.9°W, 1,360 m asl, UT, USA).

5 Materials and Methods

5.1 Field test station

A CPEC310 system was set as the core of the station in 2018. Beyond its major components briefly described in Section 4, the system also included a barometer (Model: MPXAZ6115A, Freescale Semiconductor, TX, USA) for flow pressure, pump module (SN: 1001) for air sampling, valve module (SN: 1003) to control flows for auto zero/span CO$_2$ and H$_2$O, scrub module (SN: 1002) to generate zero gas (i.e., without CO$_2$ and H$_2$O) for auto zero procedure, a CO$_2$ cylinder for CO$_2$ span, and an EC100 electronic module (SN: 1002, OS Rev 07.01) to control and measure $a_{CSAT3A}$, EC155, and a barometer. In turn, the EC100 was connected to, and instructed by, a central CR6 Datalogger (SN: 2981, OS 04) for these sensor measurements, data processing, and data output. In addition to receiving the data output from the EC100, the CR6 also controlled the pump, valve, and scrub modules and measured other micrometeorological sensors in support of this study.
The micrometeorological sensors included a LI200 pyranometer (SN: 18854, LI-COR Biosciences, Lincoln, NE, USA) to monitor incoming solar radiation, a precision platinum resistance temperature detector (RTD, model 41342, SN: TS25360) inside a fan-aspirated radiation shield (model: 43502, R.M. Young Company, Traverse City, MI, USA) to more accurately measure the temperature and humidity sensor (SN: 1073, Vaisala Corporation, Helsinki, Finland) inside a 14-plate wind-aspirated radiation shield (model 41005) to measure the temperature under conditions of potentially significant solar contamination during the day due to low wind-aspiration efficiency. The sensing centers of all sensors related to temperature, RH, and CO₂ were set at a height of 2.57 m above the ground level. The land surface was covered by natural prairie with a grass height of 5 to 35 cm.

A CR6, supported by EasyFlux CR6CP (Revised version for this study, Campbell Scientific Inc. UT, USA), controlled and sampled the EC100 at 20 Hz. For spectral analysis, the EC100 filtered the data of temperature and χH₂O for anti-aliasing using a finite impulse response filter with a 0-to-10 Hz (Nyquist folding frequency) passing band (Saramäki, 1993). The EC155 was zeroed for CO₂/H₂O and spanned for CO₂ automatically every other day and spanned for H₂O monthly using a LI-610 Portable Dew Point Generator (LI-COR Biosciences, Lincoln, NE, USA). The LI200, RTD, and HMP155A sampled at 1 Hz because of their slow response and the fact that only their measurement means were of interest to this study.

The purpose of this station was to measure the eddy-covariance fluxes to determine turbulent transfers in the boundary-layer flows. The air temperature equation \[ T \] was developed for the turbulent air flows sampled through the CPEC system. Therefore, this equation can be tested based on how the CPEC310 measures the boundary-layer flows related to turbulent transfer.

### 5.2.6 Turbulent transfer and CPEC310 measurement

In atmospheric boundary-layer flows, air constituents along with heat and momentum (i.e., air properties) are transferred dominantly by individual turbulent flow eddies with various sizes (Kaimal and Finnigan, 1994). Any air property is considered as more homogenous inside each smaller eddy and as more heterogenous among larger eddies (Stull, 1988). Due to this heterogeneity, an eddy in motion among others is transferring air properties to its surroundings. Therefore, to measure the transfer in amount and direction, a CPEC system was designed to capture temperature \( T \), χH₂O, and 3-D flow speeds from individual eddies. Ideal measurements should be fast enough to capture, although impossible, all eddies with different sizes through the measurement volume and sampling orifice of the CPEC system (Fig. 1). To capture more eddies, with as many sizes as possible, the CPEC measurements were set at a high frequency (20 Hz in this study) because, given 3-D speeds, the smaller the eddy, the shorter time the eddy takes to pass the sensor measurement volume. Ideally, each measurement captures an individual eddy for all variables of interest so that the measured values are representative of this eddy. So, for instance, in our field measurements to compute \( T \) from a pair of \( T_s \) and \( χH₂O \), the pair simultaneously measured from the same eddy could better reflect its \( T \) at the measurement time; however, in a CPEC system, \( T_s \) and \( χH₂O \) are measured with separation in both space (Fig. 1) and time (Fig. 3).

If an eddy passing the sonic anemometer is significantly larger than the dimension of separation between the \( T_s \) measurement volume and the \( χH₂O \) sampling orifice (Fig. 1), the eddy is instantaneously measured for its 3-D wind and \( T_s \) in the volume while also sampled into the orifice for \( χH₂O \) measurements. However, if the eddy is smaller and flows along the alignment of separation, the sampling takes place either a little earlier or later than the measurement, i.e., earlier if \( T_s \) is measured later, and vice versa. However, depending on its size, an eddy flowing beyond the alignment from other directions, although measured by the sonic...
anemometer, may be missed by the sampling orifice passed by other eddies and, in other cases, although sampled by the orifice, may be missed by the measurement of the sonic anemometer.

Additionally, the air flow sampled for \( \chi_{H_2O} \) measurements is not measured at its sampling time on the sampling orifice, but instead is measured, in lag, inside the \( \chi_{H_2O} \) measurement cuvette (Fig. 3). The lag depends on the time needed for the sampled flow to travel through the CPEC sampling system (Fig. 3). Therefore, for the computation of \( T_{\chi_{H_2O}} \) is better synchronized and matched with \( T_s \) as if simultaneously measured from the same eddy.

5.3.7. Temporal synchronization and spatial match for \( T_s \) with \( \chi_{H_2O} \)

In the CPEC310 system, a pair of \( T_s \) and \( \chi_{H_2O} \) that were received by CR6 from EC100 in one data record (i.e., data row) were synchronously measured, through Synchronous Device for Measurement Communication Protocol (Campbell Scientific Inc., 2018c), at the same time in the \( T_s \) measurement volume and \( \chi_{H_2O} \) measurement cuvette (Fig. 1). Accordingly, within one data row of time series received by CR6, \( \chi_{H_2O} \) was sampled earlier than \( T_s \) was measured. As discussed above, \( T_s \) and \( \chi_{H_2O} \) in the same row, although measured at the same time, might be not measured simultaneously from the same eddy. If so, the \( \chi_{H_2O} \) measurement from the same eddy of this \( T_s \) might occur in another data row, and vice versa. In any case, a logical procedure for the synchronization match is first to pair \( T_s \) with \( \chi_{H_2O} \) programmatically in CR6, as the former was measured at the same time as the latter was sampled.

5.3.1.2.4. Synchronize \( T_s \) measured to \( \chi_{H_2O} \) sampled at the same time

Among the rows in time series received by CR6, any two consecutive rows were measured sequentially at a fixed time interval (i.e., measurement interval). Accordingly, anemometer data in any data row can be synchronized with analyzer data in a later row from the eddy sampled by the analyzer sampling orifice at the measurement time of the sonic anemometer. How many rows later depends on the measurement interval and the time length of the analyzer sample from its sampling orifice to the measurement cuvette. The measurement interval commonly is 50 or 100 ms for a 20- or 10-Hz measurement frequency, respectively. The time length is determined by the internal space volume of sampling system (Fig. 3) and the flow rate of sampled air driven by a diaphragm pump (Campbell Scientific Inc., 2018a).

As shown in Fig. 3, the total internal space is 10.563 mL. The rate of sampled air through the sampling system nominally is 6.0 L min\(^{-1}\) at which the sampled air takes 106 ms to travel from the analyzer sampling orifice to the cuvette exhaust outlet (Fig. 3). Given that the internal optical volume inside the cuvette is 5.887 mL, the air in the cuvette was sampled in during a period of 47 to 106 ms earlier. Accordingly, anemometer data in a current row of time series should be synchronized with analyzer data in the next row for 10-Hz data and, for 20-Hz data, the row after that following next one. After synchronization, the CR6 stores anemometer and analyzer data in a synchronized matrix (variables unrelated to this study were omitted) as a time series:

\[
\begin{bmatrix}
  u(t_i) & v(t_i) & w(t_i) & T_s(t_i) & \chi_{H_2O}(t_i) & d_{s_i}(t_i) & d_{g_i}(t_i) & s(t_i)
\end{bmatrix},
\]

where \( u \) and \( v \) are horizontal wind speeds orthogonal to each other, \( w \) is vertical wind speed; \( d_s \) and \( d_g \) are diagnosis codes for sonic anemometer and infrared gas analyzer, respectively; \( s \) is analyzer signal strength of gas analyzer for \( H_2O \); \( t \) is time and its subscript \( i \) is its index; and the difference between \( t \) and \( t_{i+1} \) is a measurement interval \( \Delta t = t_{i+1} - t_i \). In any row of matrix (28)
(e.g., the \(i\)th row), \(t\) for anemometer data is the measurement time plus instrument lag and \(t\) for analyzer data is the sampling time plus the same lag. The instrument lag is defined as the number of measurement intervals used for data processing inside EC100 after the measurement and subsequent data communication to CR6. Regardless of instrument lag, \(T_s\) and \(\chi_{H_2O}\) in each row of synchronization matrix were temporally synchronized as measured and sampled at the same time.

### 5.3.2 Match \(T_s\) measured to \(\chi_{H_2O}\) sampled from the same eddy

As discussed in Section 5.2.6, at either \(T_s\) measurement or \(\chi_{H_2O}\) sampling time, if an eddy was large enough to enclose both \(T_s\) measurement volume and \(\chi_{H_2O}\) sampling orifice (Fig. 1), \(T_s\) and \(\chi_{H_2O}\) in the same row of synchronization matrix (28) belong to the same eddy; otherwise, they belong to different eddies. For any eddy size, it would be ideal if \(T_s\) could be spatially matched with \(\chi_{H_2O}\) as a pair for the same eddy; however, this match would not be possible for all \(T_s\) values simply because, in some cases, an eddy measured by the sonic anemometer might be never sampled by the \(\chi_{H_2O}\) sampling orifice, and vice versa (see Section 5.2.6). Realistically, \(T_s\) may be matched with \(\chi_{H_2O}\) overall with the most likelihood as many pairs as possible for a period (e.g., an averaging interval).

The match is eventually to lag either \(T_s\) or \(\chi_{H_2O}\), relatively, in the synchronization matrix (28). The lag can be counted as an integer number (\(l_s\), subscript \(s\) indicates the spatial separation causing lag) in measurement intervals where \(l_s\) is positive if an eddy flowed through the \(T_s\) measurement volume earlier, negative if later, or zero if through the \(\chi_{H_2O}\) sampling orifice at the same time. This number is estimated through the covariance maximization (Irwin, 1979; Moncrieff et al., 1997; Ibrom et al., 2007; Rebmann et al., 2012). According to \(l_s\), over an averaging interval, the data columns of the gas analyzer over an averaging interval in the synchronization matrix (28) can be moved together up \(l_s\) rows as positive, down \(l_s\) rows as negative, or nowhere as zero to form a matched matrix:

\[
\begin{bmatrix}
v_1(t) & u_1(t) & \chi_{H_2O}(t) & d_1(t) & \rho(t) & \chi_{H_2O}(t) & d_2(t) & \rho(t) & \chi_{H_2O}(t) & d_3(t) & \rho(t) & \chi_{H_2O}(t) & d_4(t) & \rho(t) & \chi_{H_2O}(t)
\end{bmatrix}
\]

(29)

For details to find \(l_s\), see EasyFlux-DL-CR6CP on https://www.campbellsci.com. In the matched matrix, over an averaging interval, a pair of \(T_s\) and \(\chi_{H_2O}\) in the same row can be assumed to be matched as if measured and sampled from the same eddy.

Using Eq. (23), the air temperature now can be computed using:

\[
T_{\text{l,ij}} = T_{\text{i,j}} \frac{1 + \epsilon \chi_{H_2O}(t)}{1 + \epsilon \chi_{H_2O}(t)} \frac{1 + \epsilon \chi_{H_2O}(t)}{1 + \epsilon \chi_{H_2O}(t)}
\]

(30)

where subscript \(l_s\) for \(T_s\) indicates that spatially lagged \(\chi_{H_2O}\) is used for computation of \(T_s\). In verification for the accuracy of equation-computed \(T_s\) and in assessments on its expected advantages of high-frequency signal insensitive to solar contamination in measurements, \(T_{\text{l,ij}}\) could minimize the uncertainties due to the spatial separation in measurements of \(T_s\) and \(\chi_{H_2O}\) between the \(T_s\) measurement volume and the \(\chi_{H_2O}\) sampling orifice (Fig. 1).
6 Results

6.1 Verification of the accuracy of equation-computed T

The accuracy of equation-computed T was theoretically specified by Eqs. (25) to (27) and was estimated in Fig. 2c. This accuracy specifies the range of equation-computed minus true T (i.e., ΔT). However, the true T was not available in the field but, as usual, precision measurements could be considered as a benchmark to represent the true T. In this study, T measured by the RTD inside a fan-aspirated radiation shield (T_RTD) was the benchmark to compute ΔT (i.e., equation-computed T minus T_RTD). If almost all ΔT values fall within the accuracy-specified range over a measurement domain of Tc and χ_H2O, the accuracy is correctly defined and the equation-computed T is accurate as specified.

To verify the accuracy over the domain as large as possible, ΔT values in the coldest (January) and hottest (July) months were used as shown in Fig. 4 (−21 °C < Tc < 35.5 °C and χ_H2O up to 20.78 mmolH2O mol−1 in a 30-minute mean over the two months). Out of 2,976 ΔT values from both months, 44 values fell out of specified-accuracy range, but near the range line within 0.30 K. The ΔT values were 0.549 ± 0.281 K in January and 0.436 ± 0.290 K in July. Although these values were almost all positively away from the zero-line due to either overestimation for Tc by the sonic anemometer within ± 1.00 K accuracy or underestimation for T_RTD by the RTD within ± 0.20 K accuracy, the ranges are significantly narrower than the specified accuracy range of equation-computed T (Figs. 2c and 4). Therefore, the equation-computed T is accurate as specified and even much better.

It is common for sonic anemometers to have a systematic error in Tc to be ±0.5 °C or a little greater, which is the reason that the ΔT accuracy is specified by Larry Jacobsen (anemometer authority) to be ±1.0 °C for the updated CSAT3A. The fixed deviation in measurements of sonic path lengths is asserted as a source for bias of Tc (Zhou et al., 2018). This bias brings an error to equation-computed T. If the T equation were not exact as Eqs. (4) and (5), there would be an additional equation error. In our study effort, this bias from fixed deviation possibly is around 0.5 °C. With this bias, the equation-computed T is still accurate as specified by Eqs. (25) to (27) and even better.
Figure 4: The error of equation-computed $T$ in coldest (January) and hottest (July) months, 2019 in Logan, UT, US. $\Delta T$ is equation-computed minus RTD-measured $T$ where RTD is a precision platinum resistance temperature detector inside a fan-aspirated radiation shield. $\Delta T$: $0.549 \pm 0.281$ K in January and $0.436 \pm 0.290$ K in July. See Fig. 2c for the accuracy range.

6.2 Assessments of the advantages of equation-computed $T$

As previously discussed, the data stream of equation-computed $T$ consists of high-frequency signals insensitive to solar contamination in measurements. Its frequency response can be assessed against known high-frequency signals of $T_s$, and the insensitivity can be assessed by analyzing the equation-computed, RTD-measured, and sensor-measured $T_i$ where the sensor is HMP155A inside a wind-aspirated radiation shield.

6.2.1 Frequency response

The matched matrix (29) and Eq. (30) were used to compute $T_{eq}$ (i.e., equation-computed $T$). Paired power spectra of equation-computed $T$ and $T_i$ are compared in Fig. 5 for three individual two-hour periods of atmospheric stratifications, including unstable ($z/L = -0.313 \sim -2.999$ where $z$ is a dynamic height of measurement minus displacement height and $L$ is the Monin-Obukhov length), near-neutral ($z/L = -0.029 \sim +0.003$), and stable ($z/L = +0.166 \sim +0.600$) atmospheric stratifications. Slower response of equation-computed $T$ than $T_i$ at higher frequency (e.g. > 5 Hz) was expected because equation-computed $T$ is derived from two variables ($T_s$ and $\chi_{H_2O}$) measured in a spatial separation, which attenuates the frequency response of correlation of two measured variables (Laubach and McNaughton, 1998), and $\chi_{H_2O}$ from a CPEC system has slower response than $T_s$ in frequency (Ibrom et al., 2007). However, the expected slower response was not found in this study. In unstable and stable atmospheric stratifications (panels a and c of Fig. 5a and 5c), each pair of power spectra almost overlap. Although they do not overlap in the near-neutral atmospheric stratification (Fig. 5b), the pair follow the same trend slightly above or below one another. In the higher frequency band of 1 to 10 Hz in panels a and b of Figs. 5a and 5b, equation-computed $T$ has a little more power than $T_i$. The three pairs of
power spectra in Fig. 5 indicate that equation-computed $T$ has a frequency response equivalent to $T$, up to 10 Hz, with a 20-Hz measurement rate considered to be a high frequency. The equivalent response might be accounted for by a dominant role of $T$ in the magnitude of equation-computed $T$. 


Figure 5: Paired comparisons of power spectra for equation-computed air temperature ($T_1$) and sonic temperature ($T_s$) at each of three atmospheric stratifications: unstable (a), near-neutral (b), and stable (c). $T_1$ and $T_s$ are equation-computed $T$ from $T_s$ and the H₂O mixing ratio of air sampled by the CPEC system through its sampling orifice in 1 lag (50 ms behind) and in -3 lags (150 ms ahead) of $T_s$ measurement; $z$ is the dynamic height of measurement minus displacement height, $L$ is Monin-Obukhov length, $S_{T_s}(f)$, $S_{T_1}(f)$ and $S_{T_{-3}}(f)$ are the power spectra of $T_s$, $T_1$ and $T_{-3}$ at $f$; and $\sigma_{T_s}^2$, $\sigma_{T_1}^2$ and $\sigma_{T_{-3}}^2$ represent the variance of $T_s$, $T_1$ and $T_{-3}$.
6.2.2 Insensitivity to solar contamination in measurements

The data of equation-computed, sensor-measured, and RTD-measured T in July, during which incoming solar radiation (Rs) in the site was strongest in a yearly cycle, are used to assess the insensitivity of equation-computed T. From the data, \( \Delta T \) is considered as an error of equation-computed T. The error of sensor-measured T can be defined as sensor-measured minus RTD-measured T, denoted by \( \Delta T_m \). From Fig. 6, \( \Delta T (0.690 \pm 0.191 \, \text{K}) \) is > \( \Delta T_m (0.037 \pm 0.199 \, \text{K}) \) when \( R_s < 50 \, \text{W m}^{-2} \) at lower radiation. However, \( \Delta T (0.234 \pm 0.172 \, \text{K}) \) is < \( \Delta T_m (0.438 \pm 0.207 \, \text{K}) \) when \( R_s > 50 \, \text{W m}^{-2} \) at higher radiation. This difference between \( \Delta T \) and \( \Delta T_m \) shows a different effect of \( R_s \) on equation-computed and sensor-measured T.

As shown in Fig. 6, \( \Delta T_m \) increases sharply with increasing \( R_s \) for \( R_s < 250 \, \text{W m}^{-2} \), beyond which it asymptotically approaches 0.40 K. In the range of lower \( R_s \), atmospheric stratification was likely stable (Kaimal and Finnigan, 1994) under which the heat exchange by wind was ineffective between the wind-aspirated radiation shield and boundary-layer flows. In this case, sensor-measured T was expected to increase with \( R_s \) increase (Lin et al., 2001; Blonquist and Bugbee, 2018). Along with \( R_s \) increase, the atmospheric boundary-layer develops from stable to neutral or unstable conditions (Kaimal and Finnigan, 1994). During the stability change, the exchange becomes increasingly more effective, offsetting the further heating from \( R_s \) increase on the wind-aspirated radiation shield as indicated by the red asymptote portion in Fig. 6. Compared to the \( \Delta T_m \) mean (0.037 K) while \( R_s < 50 \, \text{W m}^{-2} \), the magnitude of the asymptote above the mean is the over-estimation of sensor-measured T due to solar contamination.

However, \( \Delta T \) decreases asymptotically from about 0.70 K toward zero with the increase in \( R_s \) from 50 to 250 W m\(^{-2}\) and beyond, with a more gradual rate of change than \( \Delta T_m \) at the lower radiation range. Lower \( R_s \) (e.g., < 250 W m\(^{-2}\)) concurrently occurs with lower \( T_c \), higher RH, and/or unfavorable weather to \( T_c \) measurements. Under lower \( T_c \) (e.g., below 20 °C of CSAT3A manufacture conditions), the sonic path lengths of CSAT3A (Fig. 1) must become, due to thermo-contraction of sonic anemometer structure, shorter than those at 20 °C. As a result, the sonic anemometer could over-estimate the speed of sound.
(Zhou et al., 2018) and hence \( T_s \) for equation-computed \( T \), resulting in greater \( \Delta T \) with lower \( R_s \). Under higher RH conditions, dew may form on the sensing surface of six \( \text{CSAT3A} \) sonic transducers (Fig. 1). The dew, along with unfavorable weather, could contaminate the \( T_s \) measurements, resulting in greater \( \Delta T \) in magnitude. Higher \( R_s \) (e.g., \( > 250 \text{ W m}^{-2} \)) concurrently occurs with weather favorable to \( T_s \) measurements, which is the reason that \( \Delta T \) slightly decreases rather than increases with \( R_s \) when \( R_s > 250 \text{ W m}^{-2} \).

Again from Fig. 6, the data pattern of \( \Delta T > \Delta T_s \) in the lower \( R_s \) range and \( \Delta T < \Delta T_s \) in the higher \( R_s \) range shows that equation-computed \( T \) is not as sensitive to \( R_s \) as sensor-measured \( T \). The increasing trend of \( \Delta T \) with \( R_s \) increase shows the insensitivity of equation-computed \( T \) to \( R_s \). Although the purpose of this study is not particularly to eliminate solar radiation contamination, equation-computed \( T \) is indeed less contaminated by solar radiation as shown in Fig. 6.

7.4 Discussion

7.4.1 Actual accuracy

The variability of \( \Delta T \) cannot be easily evaluated. \( T_s \) measurements also possibly have a systematic error due to the fixed deviation in the measurements of sonic path lengths for sonic anemometers although the error should be within the accuracy specified in Fig. 2. A \( T_{so} \) measurement also can be erroneous if the gas analyzer is not periodically zeroed and spanned for its measurement environment. Therefore, if \( T_s \) is measured under unfavorable weather conditions, and the sonic anemometer produces a systematic \( T \) error, and if the gas analyzer is not zeroed and spanned as instructed in its manual, then the accuracy of equation-computed \( T \) would be unpredictable. Normally, the actual accuracy is better than that specified in Fig. 2. Additionally, with the improvement in measurement accuracies of sonic anemometers (e.g., weather-condition-regulated, heated 3-D sonic anemometers, Mahan et al., 2021) and gas analyzers, this accuracy of equation-computed \( T \) would be gradually becoming better and better.

For this study, filtering out the \( T_s \) data in the periods of unfavorable weather could narrow the error range of equation-computed \( T \). The unfavorable weather was suspected to contribute to the stated error. However, although filtering out unfavorable weather cases could create a lower error estimate, most field experiments include periods when weather increases a \( T \) error, so including a weather contribution to error would prevent overstating instrument accuracy under typical (unfiltered) applications. Therefore, both \( T_s \) and \( \Delta T \) data in this study were not programmatically or manually filtered based on weather.

7.4.1.2 Spatial separation of \( T_s \) and \( \Delta T_s \) in measurements

In this study, \( T_s \) was successfully computed from \( \Delta T \) and \( \chi_{so} \) as a high-frequency signal (Fig. 5) with expected accuracy as tested in Figs. 2, 4 and 6, where both were measured separately from two sensors in a spatial separation. Some open-path eddy covariance (OPEC) systems (e.g., CSAT3A+EC150 and CSAT3B+LI7500) measure \( T_s \) and \( \rho_a \) also from two sensors in a spatial separation. To OPEC systems, although the air temperature equation (Eq. 23) is not applicable, the algorithms developed
in Section 5.3.2 to temporally synchronize and spatially match $T_s$ with $\chi_{H2O}$ for computation of $T$ are applicable for computation of $T$ from $T_s$ and $\rho_d$ along with $P$ in such OPEC systems (Swiatek, 2018).

In Section 5.3.2, programming and computing are needed to pair $T_s$ measured to $\chi_{H2O}$ sampled at the same time into synchronization matrix (28) as the first step and from the same eddy into matched matrix (29) as the second step. The second requires complicated programming and much computing. To test the necessity of this step in specific cases, using Eq. (30), $T_0$ was computed from a row of the synchronization matrix and $T_{ls}$ was computed from this matrix by lagging $\chi_{H2O}$ columns up $l$, rows if $l > 0$ and down $|l|$ rows if $l < 0$ where $l$ is -5, …, -1, +1, …, +5. From the data of this study, individual $T_{ls}$ values were different for different subscript $l$, but their means for subscript $i$ over an averaging interval ($T_i$) are the same to at least the fourth digit after the decimal place. Further, the power spectrum of $T_0$ time series was compared to those of $T_{ls}$ time series, where $i \neq 0$. Any pair of power spectra from the same period overlap exactly (Figures omitted). Therefore, the second step of lag maximization to match $T_s$ measured to $\chi_{H2O}$ sampled from the same eddy is not needed if only hourly mean and power spectrum of equation-computed $T$ are of interest to computations, for both CPEC and OPEC systems.

7.3.1 Dry air density

As a high-frequency signal insensitive to solar radiation, equation-computed $T$ is more applicable than sensor-measured $T$ for calculations of $\rho_d$ and $\rho_d w$ for more applications (Gu et al., 2012; Foken et al., 2012). In practice, equation-computed $T$ may be used for $\rho_d$ and $\rho_d w$ under normal weather conditions while the sonic anemometer and gas analyzer are normally running, which can be judged by their diagnosis codes (Campbell Scientific Inc., 2018a). Under a weather condition unfavorable to $T_s$ measurements due to dew, rain, snow, and ice conditions, equation-computed $T$ from weather-condition-regulated, heated 3-D sonic anemometers (Mahan et al., 2021) and CPEC infrared gas analyzer could be an alternative. Currently, in CO$_2$, H$_2$O and trace gas flux measurements, mean $\rho_d$ for flux calculations is estimated from $T$ and RH along with $P$, $T$ and RH are measured mostly by a slow-response $T$-RH probe without fan-aspiration (e.g., IMP155A. Zhu et al., 2021).
As shown in Fig. 6, equation-computed $T$ is better than probe-measured $T$. The air moisture measured by an infrared analyzer in CPEC systems must be more accurate (Eq. (27) and Fig. 2b) than probe-measured air moisture. The better equation-computed $T$ along with more accurate air moisture has no reason not to improve the estimation for mean $\rho_d$.

### 4.2 Sensible heat flux estimated from an CPEC system

Currently, sensible heat flux ($H$) is derived from $\overline{T_w}$ with a humidity correction (van Dijk, 2002). The correction equations were derived by Schotanus et al. (1983) and van Dijk (2002) in two ways, but both from Eq. (4) derived with approximation (see Appendix A). Using the exact equation from this study, theoretically, $H$ can be more accurately estimated directly from $\overline{T_w}$, where $T$ is the equation-computed air temperature, although studies and tests for this potential application are needed. Without our exact $T$ equation, in any flux software, either Eq. (4) or (5) must to be used for sensible heat flux computation. Both equations are approximate (see Appendices A and B). Compared to either, our exact equation must be an improvement on the mathematical representation of sensible heat flux. If the equation for sensible heat flux is approximate, then even a perfect measurement gives only an approximate value for the flux.

### 4.3 RH as a high frequency signal

Conventionally, RH is measured using a temperature and humidity probe, which is unable to track the high frequency fluctuations of RH. In a CPEC system, equation-computed $T$, gas-analyzer-measured $\chi_{\text{H}_2\text{O}}$, and transducer-measured $P$ are able to catch the fluctuations in these variables at high frequency, from which RH can be computed (Sonntag, 1990; also see Appendix C). This method should provide high frequency RH, although verification is needed. Currently, the applications of high frequency properties in this RH are unknown in a CPEC system. Regardless, equation-computed $T$ provides a potential opportunity to acquire the high frequency RH for its application in the future.

### 4.4 Concluding remarks

In a CPEC flux system, the air temperature ($T$) of boundary-layer flows through the space of sonic anemometer measurement and infrared analyzer sampling (Fig. 1) is desired for high frequency (e.g., 10 Hz) with consistent representation of spatial and temporal scales for moist turbulence thermodynamics characterized by three-dimensional wind from the sonic anemometer and $\text{H}_2\text{O}/\text{CO}_2$ and atmospheric pressure from the gas analyzer measurements. High-frequency $T$ in the space can be measured using fine-wire thermocouples, but this kind of thermocouples for such an application is not durable under adverse climate conditions, being easily contaminated by solar radiation (Campbell, 1969). Nevertheless, the measurements of sonic temperature ($T_s$) and $\text{H}_2\text{O}$ inside a CPEC system are high-frequency signals. Therefore, high-frequency $T$ can be reasonably expected when computed from $T_s$ and $\text{H}_2\text{O}$-related variables. For this expectation, two equations [i.e., Eqs. (4) and (5)] are currently available. In both equations, converting $\text{H}_2\text{O}$-related variables into $\text{H}_2\text{O}$ mixing ratio analytically reveals the difference between the two equations. This difference in CPEC systems reaches ±0.18 K, bringing an uncertainty into the accuracy of $T$ from either equation and raising a question of which equation is better. To clarify the uncertainty and answer this question, the air temperature equations in terms of $T_s$ and $\text{H}_2\text{O}$-related variables are thoroughly reviewed (Sections 2 and 3; Appendices A and B). The two currently used equations [i.e., Eqs. (4) and (5)] were developed and completed with approximations (Appendices A and B). Because of the approximations, neither of their accuracies was evaluated, nor was the question answered.
Using the first principles equations, the air temperature equation in terms of $T_s$ and $\chi$ is derived without any assumption and approximation (Equation 23); therefore, the equation derived in this study does not, itself, have any error and, as such, the accuracy in equation-computed $T$ depends solely on the measurement accuracies of $T_s$ and $\chi$. Based on the specifications for $T_s$ and $\chi$ in the CPEC300 series, the accuracy of equation-computed $T$ over the $T_s$ and $\chi$ measurement ranges can be specified within ±1.01K (Figure 2). This accuracy range uncertainty is propagated mainly (±1.00 K) from the uncertainty in $T_s$ measurements (Figure 2a) and little (±0.02 K) from the uncertainty in $\chi$ measurements (Figure 2b).

Under normal sensor and weather conditions, the specified accuracy is verified based on field data as valid and actual accuracy ranges can be specified within ±1.01K (Figure 2). This accuracy range uncertainty is propagated mainly (±1.00 K) from the uncertainty in $T_s$ measurements (Figure 2a) and little (±0.02 K) from the uncertainty in $\chi$ measurements (Figure 2b).

The current applications of equation-computed $T$ in a CPEC system are to calculate dry air density ($\rho_d$) for the estimations of CO$_2$ flux ($\rho_w$CO$$_2$$w'$), where $\chi$ is CO$_2$ mixing ratio, $w'$ is vertical velocity of air, and prime indicates the fluctuation of variable away from its mean as indicated by overbar e.g., $w' = w - \bar{w}$, H$_2$O flux ($\rho_w$H$_2$O$w'$), and other fluxes. Combined with measurements of $\chi$, 3-D wind speeds, and $P$, the equation-computed $T$ can be potentially applied to the estimation of $\rho_d$ and $\rho_w$ (Gu et al., 2012; Foken et al., 2012), to the computation of high-frequency RH (Sonntag, 1990), and to the derivation of sensible heat flux ($H$) avoiding the humidity correction as needed for $H$ indirectly from $T_s$ (Schotanus et al., 1983; van Dijk, 2002).

In a CPEC flux system, although $T_s$ and $\chi$ are measured using two spatially separated sensors of sonic anemometer and infrared gas analyzer, $T_s$ was successfully computed from both measured variables as a high-frequency signal (Figure 5) with an expected accuracy (Figs. 2 and 4). Some open-path eddy-covariance (OPEC) flux systems measure $T_s$ and water vapor density ($\rho_w$) along with $P$. The algorithms developed in Section 5.32 to temporally synchronize and spatially match $T_s$ with $\chi$ for computation of $T$ are applicable to such an OPEC system to compute $T$ from $T_s$ and $\rho_w$ along with $P$. This $T$ would be a better option than sensor-measured $T$ in the system for the correction of spectroscopic effect in measuring CO$_2$ fluctuations at high frequencies (Helbig et al., 2016; Wang et al., 2016). With the improvements on measurement technologies for $T_s$ and $\chi$, particularly for $T_s$, the $T$ from our developed equation will become increasingly more accurate. Having its accuracy combined with its high frequency, this $T$ with consistent representation of all other thermodynamic variables for moist air at the spatial and temporal scales in CPEC measurements has its advanced merits in boundary-layer meteorology and applied meteorology.

Appendices

Appendix A. Derivation of Equation (4)

The sonic temperature ($T_s$) reported by a three-dimensional sonic anemometer is internally calculated from its measurements of the speed of sound in moist air ($c$) after the crosswind correction (Zhou et al., 2018), using...
where subscript \(d\) indicates dry air, \(\gamma_d\) is the specific heat ratio of dry air between constant pressure and constant volume, and \(R_d\) is gas constant for dry air (Campbell Scientific Inc., 2018b). The speed of sound in the atmospheric boundary-layer as in a homogeneous gaseous medium is well defined in acoustics (Barrett and Suomi, 1949), given by:

\[
c^2 = \frac{\gamma P}{\rho},
\]

where \(c\) is the counterpart of \(c_d\) for moist air, \(P\) is atmospheric pressure, and \(\rho\) is moist air density. These variables are related to air temperature and air specific humidity \(q\), i.e., the mass ratio of water vapor to moist air).

1. Moist air density \((\rho)\)

Moist air density is the sum of dry air and water vapor densities. Based on the ideal gas law (Wallace and Hobbs, 2006), dry air density \((\rho_d)\) is given by:

\[
\rho_d = \frac{P - e}{R_d T},
\]

where \(e\) is water vapor pressure, and the water vapor density \((\rho_w)\) is given by:

\[
\rho_w = \frac{e}{R_v T}.
\]

Therefore, moist air density in Eq. (a2) can be expressed as:

\[
\rho = \frac{P}{R_d T} \left[ 1 - \frac{e}{P} \right].
\]

Because of \(R_d/R_v = \epsilon\) (i.e., 0.622, the molar mass ratio between water vapor and dry air), this equation can be rearranged as:

\[
\rho = \frac{P}{R_d T} \left[ 1 - (1-\epsilon)\frac{e}{P} \right].
\]

Using Eqs. (a4) and (a6), the air specific humidity can be expressed as:

\[
q = \frac{\rho_w}{\rho} = \frac{\epsilon e}{P - (1-\epsilon)e}.
\]

Because of \(P >> (1-\epsilon)e\), \(q\) can be approximated as:

\[
q \approx \frac{\epsilon e}{P}.
\]

Substituting this relation into Eq. (a6) generates:

\[
\rho = \frac{P}{R_d T} \left[ 1 - \frac{1 - e}{\epsilon} q \right].
\]

2. Specific heat ratio of moist air \((\gamma)\)

The specific heat ratio of moist air is determined by two moist air properties: 1) the specific heat at constant pressure \((C_p)\) and 2) specific heat at constant volume \((C_v)\). \(C_p\) varies with the air moisture content between the specific heat of dry air at constant pressure \((C_{pd})\) and the specific heat of water vapor at constant pressure \((C_{pw})\). It must be the average of \(C_{pd}\) and \(C_{pw}\), that is, arithmetically weighted by dry air mass and water vapor mass, respectively, given by (Stull, 1988):
\[ C_p = \frac{C_{pd} \rho_d + C_{pw} \rho_w}{\rho}, \quad \text{(a10)} \]

\[ C_v = \frac{C_{vd} \rho_d + C_{vw} \rho_w}{\rho}, \quad \text{(a11)} \]

where \( C_{pd} \) is the specific heat of dry air at constant volume and \( C_{vw} \) is the specific heat of water vapor at constant volume.

Denoting \( C_{pd}/C_v \) as \( \gamma_d \), Eqs. (a10) and (a11) are used to express \( \gamma_d \) as:

\[ \gamma_d = \frac{C_{pd}}{C_v} = \frac{(1-q) + qC_{pw}/C_{pd}}{(1-q) + qC_{vw}/C_{pd}} \quad \text{(a12)} \]

3. Relate sonic temperature to air temperature

Substituting Eqs. (a9) and (a12) into Eq. (a2) leads to:

\[ c^2 = \gamma_d R_T \left( \frac{1-q}{(1-q) + qC_{pw}/C_{pd}} \right) \left[ 1 - \frac{1}{\gamma_d} \frac{\rho_d}{\rho} \right]. \quad \text{(a13)} \]

Using this equation to replace \( c^2 \) in Eq. (a1), \( T_s \) is expressed as:

\[ T_s = T \left( \frac{1-q}{(1-q) + qC_{pw}/C_{pd}} \right) \left[ 1 - \frac{1}{\gamma_d} \frac{\rho_d}{\rho} \right]. \quad \text{(a14)} \]

Given \( C_{pw} = 1.952, C_{pd} = 1.004, C_{vw} = 1.463, \) and \( C_{pd} = 717 \text{ J K}^{-1} \text{ kg}^{-1} \) (Wallace and Hobbs, 2006); this equation becomes:

\[ T_s = T \left[ 1 + 0.944223q \right] \frac{1}{\left( 1 + 1.040446q \right)} \left[ 1 - \frac{1}{1 - 0.607717q} \right]. \quad \text{(a15)} \]

Expression of the last two parenthesized terms in the right side of this equation separately as Taylor series of \( q \) (Burden and Faires, 1993) by dropping, due to \( q \ll 1 \), the second or higher terms related to \( q \) leads to:

\[ T_s = T \left[ 1 + 0.944223q \right] \left[ 1 - 1.040446q \right] \left[ 1 + 0.607717q \right]. \quad \text{(a16)} \]

In the right side of this equation, the three parenthesized terms can be expanded into a polynomial of \( q \) at the third order. Also due to \( q \ll 1 \) in this polynomial, the terms of \( q \) at the second or third order can be dropped. Further arithmetical manipulations result in:

\[ T_s = T \left[ 1 + 0.51q \right]. \quad \text{(a17)} \]

This is Eq. (4) in a different form. In its derivations from Eqs. (a1) and (a2), three approximation procedures were used from Eq. (a7) to (a8), (a15) to (a16), and (a16) to (a17). The three approximations must bring unspecified errors into the derived equation.

Appendix B. Derivation of equation (5)

Equation (5) was sourced from Ishii (1932) in which the speed of sound in moist air \( (c) \) was expressed in his Eq. (1) as:

\[ c^2 = \gamma \left( \frac{P}{\rho} \right) \left( \frac{\alpha}{\beta} \right). \quad \text{(b1)} \]
where all variables in this equation are for moist air, $\gamma$ is the specific heat ratio of moist air between constant pressure and constant volume, $P$ is moist air pressure, $\rho$ is moist air density, $\alpha$ is moist air expansion coefficient, and $\beta$ is moist air pressure coefficient. Accordingly, the speed of sound in dry air ($c_d$) is given by:

$$c_d^2 = \frac{\gamma P_d \rho_d}{P_d \rho_d} \left( \frac{\alpha_d}{\alpha_d} \beta_d \right).$$

where subscript $d$ indicates dry air in which $\gamma_d$, $P_d$, $\rho_d$, $\alpha_d$, and $\beta_d$ are the counterparts of $\gamma$, $P$, $\rho$, $\alpha$, and $\beta$ in moist air. Equations (b1) and (b2) can be combined as:

$$c^2 = c_d^2 \left( \frac{\gamma}{\gamma_d} \left( \frac{P \rho}{P_d \rho_d} \right) \left( \frac{\alpha \beta}{\alpha_d \beta_d} \right) \right).$$

Experimentally by Ishii (1932), each term inside the three pairs of parentheses in this equation was linearly related to the ratio of water vapor pressure ($e$) to dry air pressure ($P_d$). The relationship into Eq. (b3) leads to:

$$c^2 = c_d^2 \left( 1 + 0.00163 \frac{e}{P_d} \right) \left( 1 - 0.378 \frac{e}{P_d} \right)^{-1} \left( 1 - 0.0613 \frac{e}{P_d} \right).$$

Dividing by $R_d$, where $R_d$ is gas constant for dry air, over both sides of Eq. (b4) and reference Eq. (11), sonic temperature ($T_s$) is expressed in terms of air temperature ($T$), $e$, and $P_d$ as:

$$T_s = T \left( 1 + 0.00163 \frac{e}{P_d} \right) \left( 1 - 0.378 \frac{e}{P_d} \right)^{-1} \left( 1 - 0.0613 \frac{e}{P_d} \right).$$

Using the relationship of $P_0 = P - e$, this equation can be manipulated as:

$$T_s = T \left( \frac{P - 0.9984e}{P - e} \right) \left( \frac{P - 13780e}{P - e} \right)^{-1} \left( \frac{P - 10613e}{P - e} \right) = T \frac{1 - 2.0597e / P + 1.0596e / P^2}{1 - 2.3780e / P + 1.3780e / P^3}.$$ 

Dropping the second order terms due to $eP \ll 1$ in boundary-layer flows, this equation becomes:

$$T_s = T \left( 1 - 2.0597 \frac{e}{P} \right) \left( 1 - 2.3780 \frac{e}{P} \right)^{-1}.$$ 

Expanding the second parenthesized term into Taylor series and, also due to $eP \ll 1$, dropping the terms related to $eP$ at an order of second or higher, this equation becomes:

$$T_s = T \left( 1 - 2.0597 \frac{e}{P} \right) \left( 1 + 2.3780 \frac{e}{P} \right)^{-1}.$$ 

Further expanding the two parenthesized terms in the right side of this equation and dropping the second order term of $eP$ lead to:
This is Eq. (5) in a different form. From the experimental source of Eq. (b4), it was derived using three approximations from Eq. (b4) to (b7), (b7) to (b8), and (b8) to (b9). The approximations, and therefore combined uncertainty in $T_{\text{clausius}}$, bring unspecified errors into Eq. (5) [i.e., Eq. (b9)] as an equation error.

Appendix C. Water vapor mixing ratio and sonic temperature from relative humidity, air temperature, and atmospheric pressure

For a given air temperature ($T$ in °C) and atmospheric pressure ($P$ in kPa), air has a limited capacity to hold water vapor (Wallace and Hobbs, 2006). This limited capacity is described in terms of saturation water vapor pressure ($e_s$ in kPa) for moist air, given through the Clausius-Clapeyron equation (Sonntag, 1990):

$$e_s(T,P) = \begin{cases} 
0.6112 \exp\left(\frac{17.62T}{T + 24312}\right) f(P) & T \geq 0 \\
0.6112 \exp\left(\frac{22.46T}{T + 273.15}\right) f(P) & T < 0
\end{cases} \quad (c1)$$

Where $f(P)$ is an enhancement factor for moist air, being a function of atmospheric pressure: $f(P) = 1.0016 + 3.15 \times 10^{-5} P - 0.0074 P^{-1}$. At relative humidity (RH in %), the water vapor pressure ($e_{\text{RH}}(T,P)$) is:

$$e_{\text{RH}}(T,P) = \frac{RH}{100} e_s(T,P) \quad (c2)$$

Given the mole numbers of H$_2$O ($n_{\text{RH}}$) and dry air ($n_d$) at RH, the H$_2$O molar mixing ratio at RH ($X_{H_2O}^{\text{RH}}$):

$$X_{H_2O}^{\text{RH}} = \frac{n_{\text{RH}}}{n_d} = \frac{n_{\text{RH}} R^* (T + 273.15)}{n_d R^* (T + 273.15)} = \frac{e_{\text{RH}}(T,P)}{P_0} \quad (c3)$$

where $R^*$ is the universal gas constant and $P_0$ is dry air pressure. Using this equation and the relation:

$$P = P_0 + e_{\text{RH}}(T,P) \quad (c4)$$

$X_{H_2O}^{\text{RH}}$ can be expressed as:

$$X_{H_2O}^{\text{RH}} = \frac{e_{\text{RH}}(T,P)}{P - e_{\text{RH}}(T,P)} \quad (c5)$$

Using Eq. (23), this $X_{H_2O}^{\text{RH}}$ along with $T_i$ can be used to calculate sonic temperature ($T_s$) at RH, given by:

$$T_s(T, X_{H_2O}^{\text{RH}}) = (T + 273.15) \frac{1 + X_{H_2O}^{\text{RH}}}{1 + \frac{\gamma_{\rho}}{\gamma_{v}} X_{H_2O}^{\text{RH}}} \quad (c6)$$

where $\gamma_v = 0.622$ (Eq. 17), $\gamma_{\rho} = 2.04045$, and $\gamma_{v} = 1.94422$ (Eq. 23). Through Eqs. (c1) and (c2), Eqs. (c5) and (c6)
express $\chi H_{2}O$ and $T_s (T,\chi H_{2}O)$, respectively, in terms of $T$, RH, and $P$. $\chi H_{2}O$ and $T_s (T,\chi H_{2}O)$ can be used to replace $\chi_{w}$ (H₂O molar water vapor mixing ratio) and $T_s$ in Eq. (25). After replacements, Eq. (25) can be used to evaluate the uncertainty, due to $T_s$ and $\chi_{w}$, measurement accuracy uncertainties, in air temperature computed from Eq. (23) for different RH values over a $T$ range.

Author Contributions

IZ led this work; XinZ, TG, and XiaoZ derived equations, analyzed data, and drafted the manuscript; ET substantially structured and revised manuscript; and AS, TA, and JO make comments on the manuscript.

Competing interest

The authors declare that they have no conflict of interest.

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