

Article (refereed) - postprint

Ward, H.C.; Evans, J.G.; Hartogensis, O.K.; Moene, A.F.; De Bruin, H.A.R.; Grimmond, C.S.B. 2013. **A critical revision of the estimation of the latent heat flux from two-wavelength scintillometry.** *Quarterly Journal of the Royal Meteorological Society*, 139 (676). 1912-1922. [10.1002/qj.2076](https://doi.org/10.1002/qj.2076)

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A critical revision of the estimation of the latent heat flux from two-wavelength scintillometry

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Abstract

Simultaneous scintillometer measurements at multiple wavelengths (pairing visible or infrared with millimetre or radiowaves) have the potential to provide estimates of path-averaged surface fluxes of sensible and latent heat. Traditionally, the equations to deduce fluxes from measurements of the refractive index structure parameter at the two wavelengths have been formulated in terms of absolute humidity. Here, it is shown that formulation in terms of specific humidity has several advantages. Specific humidity satisfies the requirement for a conserved variable in similarity theory and inherently accounts for density effects misapportioned through the use of absolute humidity. The validity and interpretation of both formulations are assessed and the analogy with open-path infrared gas analyser density corrections is discussed. Original derivations using absolute humidity to represent the influence of water vapour are shown to misrepresent the latent heat flux. The errors in the flux, which depend on the Bowen ratio (larger for drier conditions) may be of the order of 10%. The sensible heat flux is shown to remain unchanged. It is also verified that use of a single scintillometer at optical wavelengths is essentially unaffected by these new formulations. Where it may not be possible to reprocess two-wavelength results, a density correction to the latent heat flux is proposed for scintillometry, which can be applied retrospectively to reduce the error.

Keywords: Density effects, Evaporation, Humidity, Millimetre-wave scintillometer, Refractivity

1. Introduction

There is considerable demand for reliable and accurate measurements of surface fluxes over different land surfaces to develop better understanding of land-atmosphere interactions in order to improve models and prediction capability. A key component in both water and energy balances is the evaporation, or latent heat flux. Catchment-scale information on the water balance is essential for assessing flood risk and, especially important where supplies may be limited, for managing fresh water provision (e.g. irrigation scheduling).

Two-wavelength scintillometry offers the ability to estimate the latent heat flux over large areas (e.g. 2-5 km²) (Kohsiek, 1982; Hill, 1997; Green et al., 2001; Meijninger et al., 2002; Meijninger et al., 2006). Studies have shown that measurements of turbulent heat fluxes integrated over an area of this order offer suitable comparison data for evaluating land surface schemes in numerical weather prediction models (Beyrich et al., 2002; Beyrich and Mengelkamp, 2006), hydro-meteorological models (Samain et al., 2011) or satellite retrievals of similar scales (Hoedjes et al., 2007; Kleissl et al., 2009).

Two-wavelength scintillometry requires one visible or near-infrared instrument (here referred to as optical) and another at millimetre or radio wavelengths (Andreas, 1989), positioned so that their beams are close together (Lüdi et al., 2005). The intensity fluctuations of each beam are converted into a measure of the refractive index fluctuations of air at the corresponding wavelength using turbulence and wave propagation theory (Tatarski, 1961; Wheelon, 2006). The quantity retrieved is the path-averaged refractive index structure parameter, C_n^2 (Wang et al., 1978). At optical wavelengths the refractive index fluctuations are almost entirely due to temperature fluctuations, whereas longer wavelengths have greater sensitivity to humidity fluctuations.

For each wavelength C_n^2 can be written in terms of temperature (C_T^2) and humidity (C_q^2) structure parameters and the cross-structure parameter (C_{Tq}). Solving simultaneously yields the contributions from temperature and humidity, using the two measured values of C_n^2 plus an estimate of the temperature-humidity correlation coefficient r_{Tq} (Hill et al., 1988). Alternatively the cross-structure parameter can be found directly by correlating the signals at each wavelength: this bichromatic method enables the correlation between temperature and humidity to be measured and thus removes the need to assume a value for r_{Tq} (Beyrich et al., 2005; Lüdi et al., 2005). Monin-Obukhov Similarity Theory (MOST) is then used to calculate the scaling variables of temperature and humidity, from which sensible and latent heat fluxes are found (Kohsiek, 1982; Hill, 1997; Green et al., 2001; Meijninger et al., 2002; Meijninger et al., 2006).

Previously, the absolute humidity (Q , i.e. the mass of water vapour per volume of moist air, kg m^{-3}) has been used to represent the water vapour content of the atmosphere. The original derivations (Hill et al., 1980; Andreas, 1988) partitioned the refractive index fluctuations into temperature fluctuations and absolute humidity fluctuations. Hill (1989) uses absolute humidity to derive structure parameters and scaling variables; Kohsiek (1982), Kohsiek and Herben (1983), Hill et al. (1988), Green et al. (2001), Meijninger et al. (2006) and Evans (2009) all employ absolute humidity in the calculation of the latent heat flux, denoted $L_v E$, where L_v is the latent heat of vaporisation and E is the evaporation. Possibly the use of Q in these studies is because Wyngaard and Clifford (1978) stated that $E = \overline{w'Q'}$ (where w' represents fluctuations in vertical wind speed). This is not always correct, especially for high Bowen ratio (β , turbulent sensible to latent heat flux ratio) conditions. Wesely (1976), one of the first to suggest deriving fluxes from scintillometry, used water vapour pressure (e , Pa).

Unfortunately, the symbols used in the literature are not consistent. Nevertheless, specific humidity $q (= Q/\rho, \text{kg kg}^{-1}$, where ρ is the density of moist air, kg m^{-3}) has been little used in the two-wavelength literature. Tatarski (1961, page 55) first expressed the refractive index in terms of the potential temperature and specific humidity, because these are conserved additives. Hill (1997) and Moene (2003) remark that conserved quantities (i.e. potential temperature and specific humidity) should be used in MOST. In Hill's (1997) detailed discussion of two-wavelength algorithms, the structure parameters C_Q^2 and C_{TQ} are obtained from C_n^2 and then converted to C_q^2 and C_{Tq} for use in MOST, but he gives the latent heat flux in terms of the absolute humidity scaling variable, Q^* . Hill (1978) provides a good discussion on the conservation of different humidity variables.

Here we argue that specific humidity should be used in two-wavelength scintillometry: firstly, it is independent of temperature; secondly, it is conserved, thus suitable for use in MOST; and thirdly, it is an appropriate variable to use to estimate the latent heat flux. Whilst Q is defined with respect to a volume, which changes with temperature (due to thermal expansion) or pressure fluctuations of vertical motions, q uses relative densities (mass of water vapour per mass of moist air). Thus specific humidity is considered a conserved quantity (Lee and Massman, 2011) in the lower part of the atmosphere (for dry adiabatic processes) whereas Q is not. Since the latent heat flux is concerned with the transport of water vapour it is necessary to avoid contamination through changes in temperature.

Figure 1 provides an overview of the processing stages discussed. The surface moisture flux can be obtained from measured C_n^2 via two paths, using either specific humidity (route a) or absolute

humidity (route b), although as will be shown here, route b is not recommended. Previously, step 1b has been used to find C_Q^2 , usually followed by 2b and 3b. The main source of error is from following the b route and taking u_*Q_* as the evaporation (i.e. stopping after 3b) which is incorrect. Additionally, step 2b is not strictly valid. Errors also arise from inconsistency, such as mistakenly arriving at C_q^2 after applying 1b.

As Q contains temperature information, it is not an ideal measure of humidity. C_q^2 is a useful statistic to describe fluctuations in water content, whereas C_Q^2 is contaminated by temperature fluctuations. The requirements for MOST scaling are satisfied by q_* (but not necessarily Q_*). Thus q_* is a much more appropriate variable to use to estimate the latent heat flux and properly account for density effects.

Since ρ depends on the water vapour content (relative molecular mass of moist air decreases with water vapour content), the resulting $L_v E$ is usually slightly underestimated when the mass of water vapour is considered relative to moist air. That is, even when using q , a small density effect occurs due to the latent heat flux itself. Bakan (1978) concluded that the most suitable quantity to determine the latent heat flux is the mass mixing ratio relative to the density of dry air ($r = Q/\rho_d$, kg kg⁻¹, where ρ_d is the density of dry air). Scintillometry data could be processed using r , yielding the structure parameter of mixing ratio (C_r^2) and $L_v E$ found from a scaling variable of mixing ratio (r_*). In practice other uncertainties in the measurements, processing and assumptions in the derivation of equations outweigh the difference between using r or q , for example instrumental noise, absorption and limitations of MOST (Medeiros Filho et al., 1983; Meijninger et al., 2006; Beyrich et al., 2012). Mixing ratio formulations are given in the Appendix.

The objective of this paper is to present the key scintillometry equations in terms of the specific humidity, giving the formulations necessary to calculate specific humidity structure parameters and correctly estimate latent heat fluxes. Section 2 outlines the theory, comparing the use of q and Q . Equations to correctly calculate the latent heat flux from two-wavelength scintillometry are given and the analogy with other measurement techniques is made in Section 3. In light of these findings, recommendations are given for processing and analysis (Section 4), implications are discussed (Section 5) and conclusions drawn (Section 6). Note that only the real part of the refractive index fluctuations is considered here (i.e. no absorption).

2. Scintillometry theory re-examined

2.1. Formulating the refractive index

Following Hill et al. (1980) and Andreas (1988), the refractive index (n) can be expressed as refractivity, defined as $10^6(n-1)$, and related to the contributions from dry air (n_d) and water vapour (n_v),

$$10^6(n-1) = n_d + n_v = m_1 \left[\frac{p-e}{T} \right] + m_2 \frac{e}{T}, \quad (1)$$

where p is the atmospheric pressure (Pa) and T air temperature (K). The values of m_1 and m_2 have been found empirically and are given by Owens (1967) for wavelengths (λ) in μm :

$$m_{1_opt} = 0.237134 + \frac{68.39397}{130 - \lambda^{-2}} + \frac{0.45473}{38.9 - \lambda^{-2}} \quad (2a)$$

$$m_{2_opt} = 0.648731 + 0.0058058\lambda^{-2} - 0.000071150\lambda^{-4} + 0.000008851\lambda^{-6} \quad (2b)$$

for optical wavelengths ($0.36 > \lambda_{opt} > 3 \mu\text{m}$). For millimetre wavelengths ($\lambda_{mw} > 3 \text{ mm}$) (Bean and Dutton, 1966):

$$m_{1_mw} = 0.776 \quad (3a)$$

$$m_{2_mw} = m_{2a_mw} + m_{2b_mw}(T) = 0.720 + \frac{3750}{T}. \quad (3b)$$

For optical wavelengths the refractivity is wavelength dependent through m_{1_opt} and m_{2_opt} , whereas there is no wavelength dependence in the millimetre range but m_{2_mw} depends inversely on T .

Contrary to Hill et al. (1980) and Andreas (1988), who used absolute humidity, we use the ideal gas law to rewrite the vapour pressure (e) in terms of the specific humidity:

$$10^6(n-1) = m_1 \frac{p}{T} + (m_2 - m_1) R_v \frac{pq}{RT}. \quad (4)$$

R is the specific gas constant for moist air: $R = R(q) = R_d + q(R_v - R_d)$ with R_d and R_v the specific gas constants for dry air and water vapour, respectively. This stage differs from the original derivations which substituted e/T as $R_v Q$ (ideal gas law). We reformulate this in terms of specific humidity ($R_v \rho q$)

and write the density as p/RT to obtain n as a function of T , q , and p . Thus for millimetre wavelengths:

$$10^6(n_{mw} - 1) = 0.776 \frac{p}{T} + (0.720 + \frac{3750}{T} - 0.776)R_v \frac{pq}{RT}. \quad (5)$$

This was first presented by Hartogensis and Moene (2011). Moene et al. (2004) give the specific humidity formulation for optical wavelengths.

2.2. Re-derivation of structure parameter coefficients

Equation 4 expresses the refractive index in terms of three variables (T , q and p), recalling that the gas constant for moist air is a function of q . Thus the change in n can be written in terms of partial derivatives:

$$\partial n = \frac{\partial n}{\partial T} \partial T + \frac{\partial n}{\partial q} \partial q + \frac{\partial n}{\partial p} \partial p, \quad (6)$$

where each derivative is found while holding the other variables constant. If the absolute humidity is used, the differentiation with respect to T , for example, creates the artificial situation of a temperature change which is forbidden from changing Q , whereas a parcel of moist air will expand when warmed, causing Q to decrease. The use of specific humidity avoids this as T and q are independent variables.

Considering relative changes in T , q and p , (6) can be re-written

$$n' = A_t \frac{T'}{T} + A_q \frac{q'}{q} + A_p \frac{p'}{p} \quad (7)$$

with primes indicating fluctuations, overbars indicating mean values, and the structure parameter coefficients defined for a scalar, y , as

$$A_y = \bar{y} \frac{\partial n}{\partial y}. \quad (8)$$

The humidity variable chosen results in different coefficients for specific (A_t , A_q) or absolute humidity (A_T , A_Q). The difference in the coefficients for temperature occurs due to the definition (8): for the derivation in terms of absolute humidity, A_T is formed from the partial differential of n with respect to T at constant absolute humidity; if specific humidity is used then A_t is obtained from the partial differential of n with respect to T at constant specific humidity. Note that A_T and A_t are both derivatives with respect to temperature, whereas A_Q and A_q are derivatives with respect to absolute

and specific humidity respectively. Following the same convention, in the case of the mass mixing ratio A_r is formed from the partial derivative of n with respect to T at constant mass mixing ratio and A_r from the partial derivative with respect to r at constant temperature, see Appendix.

As for the original derivations, pressure terms are not included (Andreas, 1988; Hill, 1997). Following Moene et al. (2004), who demonstrated that pressure fluctuations are negligible for optical wavelengths, we conclude that they can also be ignored for millimetre wavelengths. Table 1 compares the magnitude of each term in (7). Small relative fluctuations in p mean the pressure terms usually remain small enough to be ignored. This is also fortunate, since the two-wavelength method relies on a pair of simultaneous equations to solve for the two unknowns – temperature and humidity fluctuations (Hill et al., 1988).

The explicit forms of the structure parameter coefficients are given in Table A1 (Appendix) and illustrated in Figure 2. When formulated in terms of specific humidity the coefficients gain additional terms due to the presence of T in the density ($\rho = p/RT$). For optical scintillometry, the difference between absolute and specific humidity formulations is negligible as nearly all refractive index fluctuations are caused by temperature variations and humidity plays a very small role (Figure 2a). The additional terms (Table A1) contribute less than 1% to the structure parameter coefficients. Therefore for single-wavelength (optical or near-infrared) scintillometry, the effect of the choice of humidity variable is practically negligible. However, for longer wavelengths, A_q is very slightly smaller than A_Q (again $< 1\%$) but the magnitude of A_r is about 20% larger (more negative) than A_T under typical atmospheric conditions. This arises mostly from the additional differentiation of the n_{v_mw} term with respect to T when specific humidity is used (arrow, Figure 2a). The dependence of m_{2_mw} on temperature coupled with the representation of specific humidity requiring a $1/T$ dependence is responsible for this term appearing twice in A_r compared to the same term appearing once in A_T .

The sizes of the structure parameter coefficients vary with atmospheric conditions (Figure 2b). The temperature is relevant for optical wavelengths (higher T results in less negative A_T and A_r) but both temperature and humidity affect the structure parameter coefficients for the millimetre region. Smaller Q results in smaller absolute values of the temperature and humidity structure parameter coefficients (compare coefficients for decreasing relative humidity (RH) at constant temperature) and a smaller difference between absolute and specific humidity formulations: A_r is 8% larger than A_T for a relative humidity of 30% ($Q = 0.0038 \text{ kg m}^{-3}$ at $T = 288 \text{ K}$). At constant RH, increasing T is accompanied by larger Q and an increase in the magnitude of the millimetre wavelength structure parameter coefficients (and a larger difference between A_r and A_T), whereas the magnitudes of

optical A_t and A_T decrease. Pressure has a small effect: $\pm 5 \times 10^3$ Pa variation alters the difference between millimetre A_t and A_T by less than 1%.

The layout of Table A1 and Figure 2a is intended to aid comparison between Q and q formulations. The q formulation can be found for the optical region in Moene et al. (2004) but has not previously been given in the literature for millimetre wavelengths. The mixing ratio formulations are not known to have been presented before. The most useful structure parameter coefficients, A_t and A_q , are summarised in Table 2 with simplified notation so that both wavelength regions have the same general form. This is intended to be a reference, and as such shows the full expressions.

2.3. Structure parameter relations and the interpretation of structure parameters

Critically, the alternative structure parameter coefficients relate to *different* structure parameters. C_n^2 can be written using the general definition of the structure parameter for a scalar y (Monin and Yaglom, 1971),

$$C_y^2 = \overline{(y'(x) - y'(x + \delta))^2} \delta^{-2/3}, \quad (9)$$

where x is location and δ is the separation distance. Substituting (7) into (9) and tidying the right hand side gives

$$C_n^2 = \frac{A_t^2}{T^2} C_T^2 + 2 \frac{A_t A_q}{T q} C_{Tq} + \frac{A_q^2}{q^2} C_q^2. \quad (10)$$

The structure parameters obtained here are C_{Tq} ($\text{K kg kg}^{-1} \text{ m}^{-2/3}$) and C_q^2 ($\text{kg}^2 \text{ kg}^{-2} \text{ m}^{-2/3}$), which are clearly different physical quantities to C_{TQ} ($\text{K kg m}^{-3} \text{ m}^{-2/3}$) and C_Q^2 ($\text{kg}^2 \text{ m}^{-6} \text{ m}^{-2/3}$). Although the coefficients A_T and A_t are different, C_T^2 is the same whether the derivation uses absolute or specific humidity. The difference in structure parameter coefficients is compensated for by the fundamental differences in the structure parameters of humidity (C_Q^2 compared to C_q^2) and cross-structure parameters (C_{TQ} compared to C_{Tq}). Both methods separate the refractive index fluctuations into contributions from temperature, humidity and correlated temperature-humidity fluctuations, however, the meaning of humidity fluctuations is not the same, as illustrated by using the ideal gas law to relate changes in q to changes in Q . From the definition of q and the ideal gas law

$$q = \frac{QRT}{p}. \quad (11)$$

Using Reynolds decomposition and keeping only first order terms, the fluctuations in Q can be written (see Hill (1997) for details)

$$\frac{Q'}{Q} = \frac{q'}{\gamma q} - \frac{T'}{T} + \left(\frac{p'}{p} \right), \quad (12)$$

where γ is R/R_d . Neglecting pressure fluctuations (column 4, Table 1) and using (9), the structure parameter for absolute humidity can be written in terms of the structure parameters for the independent variables of temperature and specific humidity:

$$\frac{C_Q^2}{Q^2} = \frac{C_q^2}{\gamma^2 q^2} + \frac{C_T^2}{T^2} - 2 \frac{C_{Tq}}{\gamma T q}. \quad (13)$$

Hill (1997) gives the specific parameters in terms of the absolute parameters (and also the cross-structure parameter) in his Equations 14a, b:

$$\frac{C_q^2}{\gamma^2 q^2} = \frac{C_Q^2}{Q^2} + \frac{C_T^2}{T^2} + 2 \frac{C_{TQ}}{TQ} \quad (14)$$

and

$$\frac{C_{Tq}}{\gamma T q} = \frac{C_T^2}{T^2} + \frac{C_{TQ}}{TQ}. \quad (15)$$

The additional $1/T$ on the left of (15) is believed to be missing in Hill (1997). These equations clearly show that the partitioning of temperature and humidity fluctuations varies between the specific and absolute approach. Substituting (14) and (15) into (10) recovers the more familiar C_n^2 equation (with A_T and A_Q , C_T^2 , C_Q^2 and C_{TQ}). Both absolute and specific humidity structure parameters are valid in their own right – but C_Q^2 can be non-zero even when there is no evaporation.

In order to calculate heat fluxes from C_n^2 at both wavelengths, we first calculate structure parameters via the two-wavelength methodology given in Hill (1988). Both the original absolute humidity formulation and the new specific humidity route are evaluated here. We assume $C_{Tq} = r_{Tq}(C_T^2 C_q^2)^{1/2}$ with $r_{Tq} = \pm 1$, and likewise for Q . To demonstrate differences between the two approaches, heat fluxes are calculated using MOST which requires parameter specification. The

following arbitrary values for demonstration are used: a measurement height of 10 m, roughness length of 0.01 m and wind speed of 10 m s⁻¹. The Andreas (1988) stability functions are used, with identical functions assumed for temperature and humidity. Unless otherwise stated $T = 288$ K, $p = 10^5$ Pa and $Q = 0.012$ kg m⁻³ (typical values from Meijninger (2003)). To represent different atmospheric conditions available energies of 500 W m⁻² and -50 W m⁻² are shown as examples of day and night time energy regimes. The optical wavelength used throughout is 0.880 μ m.

Figure 3a illustrates the contributions of each term in (10) to the total millimetre-wavelength C_n^2 for the absolute and specific humidity formulations. As discussed, C_T^2 is the same in each case and the difference between $(A_T^2/T^2)C_T^2$ and $(A_i^2/T^2)C_T^2$ is due to the structure parameter coefficients. The contributions of humidity and temperature-humidity fluctuations to C_n^2 are different between the two approaches, due to both a difference in structure parameter coefficients and the structure parameters themselves. Figure 3b shows the difference between C_q^2 and C_Q^2 (divided by $\bar{\rho}$ to obtain compatible units).

It should be noted that the two-wavelength approach does not yield a single unique solution as there is an ambiguity in the sign of the cross-structure term (Hill et al., 1988; Hill, 1997), resulting in two possible Bowen ratios for a given C_n^2 (solid line in Figure 3a). Applications of the two-wavelength method to date reported in literature (Kohsiek, 1982; Hill, 1997; Green et al., 2001; Meijninger et al., 2002; Meijninger et al., 2006) refer to conditions where β is to the left of the C_n^2 minimum (Figure 3a). For drier conditions (i.e. higher β) it is more difficult to select the correct solution without additional information on the true value of β , either from other measurements such as eddy covariance or site characteristics. It is outside the scope of this paper to discuss in detail this feature. However the bichromatic method offers the key advantage of providing a measurement of C_{Tq} (Lüdi et al., 2005) so the sign ambiguity is not relevant.

2.4. Similarity theory scaling

Monin-Obukhov Similarity Theory is the required mechanism to establish fluxes from scintillometry measurements. It uses dimensionless relations to parameterise the variability of atmospheric quantities based on empirically derived profiles and the surface fluxes. A prerequisite for MOST is that the quantity being modelled is a conserved scalar.

Strictly, potential temperature should be used in similarity theory, but if pressure fluctuations are neglected then potential temperature changes are proportional to temperature changes and this does not create a problem (Hill, 1997). However, as absolute humidity is not a conserved variable it is not necessarily suitable for use with MOST scaling. Despite its prevalence in the literature, it is

therefore questionable to apply MOST to C_Q^2/Q_*^2 as noted by Moene (2003) and Hill (1997). Furthermore, if the intention is to study scaling relations, in particular whether heat and moisture behave similarly (e.g. Kohsiek (1982), Roth and Oke (1995), Moene and Schüttemeyer (2008)), it is preferable to compare independent measures (T and q) as in Kohsiek and Bosveld (1987), De Bruin et al. (1993) and Li et al. (2012), rather than use Q which contains an inherent T dependence. Although errors in misapplying MOST to Q may be small (especially compared to e.g. assuming identical functions for temperature and humidity), the propagation of the temperature fluctuations through C_Q^2 to Q_* is a more significant issue (discussed in Section 2.5).

2.5. Formulation of the latent heat flux

We determine the latent heat flux based on u_*q_* rather than u_*Q_* (Hill, 1997; Green et al., 2001; Meijninger et al., 2006) where u_* is the friction velocity. According to Webb et al. (1980), the water vapour mass flux is given by

$$E = -\frac{\bar{\rho}}{(1-q)} \overline{w'q'} \quad (16)$$

to a close approximation. Analogously, to estimate the latent heat flux from two-wavelength scintillometry via scaling variables, one should use

$$L_v E = -\frac{\bar{\rho}}{(1-q)} L_v u_* q_*. \quad (17)$$

The $(1-q)^{-1}$ factor arises because the water vapour flux itself causes a density change, as detailed in Webb et al. (1980) and mentioned in Section 1. When the latent heat flux is positive, $L_v E$ derived from absolute humidity ($-L_v u_* Q_*$) is expected to be an underestimate of the true flux for positive sensible heat flux (H) and an overestimate for negative H . These conclusions follow from (12) when multiplied by w' and averaged. The underestimation of the latent heat flux increases with increasing H . The magnitude of a negative latent heat flux will be underestimated by a negative H and overestimated by a positive H . This means that for positive β the magnitude of $L_v E$ is underestimated and for negative β it is overestimated.

Figure 4a shows the sensible and latent heat fluxes obtained using both humidity methods as a function of Bowen ratio. The sensible heat flux is unaffected by the choice of humidity variable (grey hollow and filled shapes are coincident). However, for unstable conditions ($H > 0$) and positive β , the latent heat flux calculated using the absolute humidity ($-L_v u_* Q_*$) can considerably underestimate the true latent heat flux calculated from (17). If H is negative but $L_v E$ is positive, $-L_v u_* Q_*$ overestimates

$L_v E$. Such conditions may occur in the nocturnal boundary layer with small available energies (squares) or during daytime over a wet surface (De Bruin et al., 2005) with larger available energies (circles). The biggest differences between absolute and specific formulations of the latent heat flux occur when the magnitude of the sensible heat flux is largest (i.e. at large Bowen ratios). The percentage error in latent heat flux is plotted in Figure 4b. At low Bowen ratios the effect is small to negligible ($< 5\%$ for $\beta < 0.5$); at higher Bowen ratios the correction becomes appreciable ($> 10\%$ for $\beta > 1.0$). The small underestimation visible at low β is due to the density effect caused by the latent heat flux itself (Section 1).

With $\beta = 1$ and an available energy of 500 W m^{-2} ($H = L_v E = 250 \text{ W m}^{-2}$) the absolute humidity method yields 225 W m^{-2} , i.e. an underestimation of 25 W m^{-2} or 10% . When $\beta = 3$ ($H = 375 \text{ W m}^{-2}$, $L_v E = 125 \text{ W m}^{-2}$) the larger sensible heat flux gives rise to a greater underestimation, with $-L_v u_* Q_* = 91 \text{ W m}^{-2}$, which translates as an absolute error of 34 W m^{-2} and a percentage error of 27% . The percentage error in the latent heat flux increases with the size of β (Figure 4b), but it must be noted that the total latent heat flux also decreases with increasing β for a given available energy (e.g. a 23% error corresponds to a smaller absolute error of 5.6 W m^{-2} at $\beta = -3$, $H = -75 \text{ W m}^{-2}$, $L_v E = 25 \text{ W m}^{-2}$). With respect to atmospheric conditions, the percentage error is largest for higher T and RH, whilst changes in p have a smaller effect (not shown). For Figure 4b a wide range of T , RH and p is shown so for most setups the variation encountered will be much smaller than indicated here. The percentage error is unaffected by stability, site characteristics or wind speed – the curves in Figure 4a collapse onto the single solid line in Figure 4b. The error depends on the partitioning of H and $L_v E$ and is affected by T , Q and p (Section 3).

3. Density corrections for open-path gas analysers

The conclusions reached in Section 2 are in accordance with the key ideas of the Webb et al. (1980) (WPL) correction for latent heat flux measured by open-path gas analysers in combination with sonic anemometers. In the eddy covariance method, fast-response gas density and temperature measurements are combined with fast-response vertical wind speed observations. The sensible and latent heat fluxes obtained are proportional to the covariances of the vertical wind speed with temperature and humidity respectively (MOST is not required). Open-path gas analysers measure absorption of radiation, which is proportional to the density of a gas, e.g. the absolute humidity. The latent heat flux is obtained from $\overline{w'Q}$ but this must be corrected for density effects using the WPL correction before a true latent heat flux measurement can be obtained.

Both gas analysers and scintillometers effectively sense changes in density along an optical (or millimetre wavelength) path. If the density measurement is expressed in terms of the absolute humidity, this will suffer the influence of temperature and water vapour fluctuations and either $\overline{w'Q'}$ (for eddy covariance) or u_*Q_* (for scintillometry) will require a correction to account for the difference from the true latent heat flux. If specific humidity is used ($\overline{w'q'}$ or u_*q_*), the difference is almost zero, with only a small correction for water vapour required – of the order of $(1-q)^{-1}$, as appears in (16) and (17).

When data cannot be reprocessed from measured C_n^2 values, it is useful to have a correction to the latent heat flux calculated from u_*Q_* to account for density effects using a WPL-style correction. The evaporation may be expressed as

$$E = -\frac{\overline{\rho}}{(1-q)}u_*q_* = -(1 + \frac{\overline{Q}}{\rho_d} \frac{R_v}{R_d})(u_*Q_* + \frac{\overline{Q}}{T}u_*T_*), \quad (18)$$

which is very similar to the familiar WPL form (Equation 25 of Webb et al. (1980)). When corrected for density effects via (18), the absolute formulation agrees with (17) (solid lines in Figure 4a).

The Bowen ratio should be specified in terms of specific humidity,

$$\beta = \frac{H}{L_v E} = (1-q) \frac{-\overline{\rho} c_p u_* T_*}{-\overline{\rho} L_v u_* q_*} = (1-q) \frac{c_p}{L_v} \frac{T_*}{q_*}, \quad (19)$$

where c_p is the specific heat capacity of air at constant pressure, so that when T and q are assumed to obey the same similarity scaling,

$$\beta = \pm(1-q) \frac{c_p}{L_v} \sqrt{\frac{C_T^2}{C_q^2}} \approx \pm \frac{c_p}{L_v} \sqrt{\frac{C_T^2}{C_q^2}}. \quad (20)$$

Combining (18) and (19), the error in the latent heat flux can be found as a function of Bowen ratio,

$$\left(1 - \frac{u_*Q_*}{\frac{\overline{\rho}}{(1-q)}u_*q_*} \right) \times 100\% = \left(1 - \frac{1}{(1 + \frac{\overline{Q}}{\rho_d} \frac{R_v}{R_d})} + \frac{\overline{Q}}{T} \frac{L_v}{\rho c_p} \beta \right) \times 100\%, \quad (21)$$

shown in Figure 4b.

Although the form of the correction to find $L_v E$ is analogous to the WPL correction for eddy covariance (Webb et al., 1980), it does not rely on vertical wind speed. Lee and Massman (2011) present a derivation of the corrections for density fluctuations (for trace gas measurements by eddy covariance) founded on the ideal gas law. Therefore, it becomes apparent that WPL is not confined to eddy covariance but, when using Q , is a necessary consideration to properly account for density changes in the humidity variable measured.

4. Recommendations

The fact that absolute humidity is not conserved formally precludes its use in MOST and this alone means it is not a suitable variable for obtaining fluxes via similarity scaling. Therefore either a composite method as set out in Hill (1997), where C_Q^2 is converted to C_q^2 for use in MOST to find q_* , can be used; or the new structure parameter coefficients presented here (Table 2) can be applied and the data processed entirely using specific humidity formulations. Note that where Hill's (1997) method has been followed, the final stage of computing the latent heat flux differs from the argument presented here (he converts back to Q_* in order to find $-L_v u_* Q_*$). It is noted here that all published two-wavelength scintillometry estimates of the latent heat flux appear to contain this error, which has not been recognised before. To correctly account for the density effects (17) should be used instead.

Ideally, the specific humidity should be used throughout the calculations. When scintillometric fluxes have been calculated based on absolute humidity and it is not possible to reprocess the data, then the density correction (18) should be applied retrospectively. This will allow interpretation of published results, as often it may be possible to approximately correct the latent heat flux using the information contained within the publication. Although this still incorporates Q_* obtained using an inappropriate method (MOST for a non-conserved quantity) these errors may be small when similarity functions for temperature and moisture are almost identical.

To summarise (Figure 1), if route 1b is used to find C_Q^2 , this can be converted to C_q^2 via 1c or Q_* to q_* via 2c. In principle MOST requires conserved variables, making 2b invalid, although under perfect MOST conditions T - q similarity is obeyed and 2a and 2b would become equivalent. Taking $u_* Q_*$ as the evaporation gives an inaccurate estimation of the evaporation and the WPL-style correction of Equation 18 should be applied to find the true value (step 3c). However, the recommended route is to use specific humidity throughout, following route 1a, 2a and 3a, in order to estimate the surface moisture flux from measured C_n^2 .

5. Implications

It has been shown here that the widespread use of absolute humidity in latent heat fluxes derived from two-wavelength scintillometry will likely result in an error in the estimation of the true latent heat flux. For campaigns over agricultural land, such as the Flevoland (Meijninger et al., 2002) and LITFASS (Meijninger et al., 2006) experiments, Bowen ratios were generally low (< 1), suggesting an underestimation of a few percent, but this will be larger (perhaps 10%) for drier fields. Future two-wavelength observations over areas with larger β would be expected to show a greater discrepancy.

Formulating the refractive index in terms of specific rather than absolute humidity changes how that measurement is interpreted. However the C_n^2 measurement itself is unchanged. Therefore the recommendations made here do not alter the effective height scaling method as outlined in Evans and De Bruin (2011), which is based around the effective measurement height of C_n^2 and occurs before the partitioning of refractive index fluctuations into temperature and humidity contributions.

Through the choice of humidity variable, it may appear that the instrument sensitivity to humidity fluctuations has changed. However, this is not the case – it is simply that the sensitivity to specific humidity is more relevant than the sensitivity to absolute humidity. The suitability of different wavelength combinations (such as the three-wavelength method (Andreas, 1990) or the two-wavelength analysis (Andreas, 1991)) could be reformulated using q . The reduced C_n^2 sensitivity of millimetre-wave scintillometers at certain Bowen ratios ($\beta \approx 2-3$), brought about by the negative C_{Tq} term and noted by Otto et al. (1996), cannot be avoided by choosing to work with specific rather than absolute humidity (Figure 3a). Further research is required on this topic.

At optical wavelengths the choice of specific or absolute humidity makes little difference because at those wavelengths the fluctuations are almost entirely due to temperature variation. Fortunately, this means that the single-wavelength scintillometry equations are not noticeably different between humidity variables ($< 1\%$ difference in structure parameter coefficients) and no changes are necessary for the single-wavelength method. Furthermore, with a single scintillometer setup the latent heat flux is estimated from the surface energy balance. Thus neither the sensible nor latent heat fluxes estimated from single-wavelength scintillometry require significant adjustment as a result of the work presented here.

6. Conclusions

Through re-examination of the methodology to estimate the latent heat flux from two-wavelength scintillometry it is concluded that the common use of absolute humidity is not advised for two main reasons: (a) Q is not a conserved variable and so should not be used in MOST, and (b) changes in Q are not independent of changes in temperature. The latter is more significant: not accounting for density effects can result in an underestimation of the daytime latent heat flux by more than 20% for very dry conditions, and around 5-15% for more typical conditions.

The use of specific humidity to represent the water vapour content of the atmosphere overcomes both issues; it is a conserved variable and independent of temperature. Importantly, changes in specific humidity are related to a surface source or sink of water molecules and cannot arise solely from variations in temperature. After re-deriving the central equations required to process scintillometry data in terms of q , different structure parameters are obtained (C_q^2 and C_{Tq}) leading to the scaling variable of specific humidity (q_*). The latent heat flux is then calculated using q_* , ensuring that a temperature change alone cannot give rise to an apparent latent heat flux. The resulting flux properly accounts for density effects due to temperature, and by including the $(1-q)^{-1}$ factor in accordance with Webb et al. (1980), the additional small correction for the water vapour flux is applied.

The new formulation for the latent heat flux is in accordance with the open-path eddy covariance work in Webb et al. (1980). For scintillometry there is the advantage of being able to choose to work with q at an early stage. It is recommended to use specific humidity throughout so density effects and MOST requirements are inherently taken care of. By working with independent variables, it is possible to separate the influences of temperature and water vapour. Most critically, this ensures comparisons can be made with other measurement techniques, model output or theoretical predictions.

Accounting for density effects enables correct calculation of the latent heat flux. For positive β , the true latent heat flux obtained is greater than the estimate obtained if density effects have not been properly accounted for through use of the absolute humidity. Previous studies have tended to indicate that latent heat fluxes estimated from scintillometry are already quite high (Green et al., 2000), perhaps suggesting there are other problems with the methodology or instrumentation that have not been considered. In order to progress, the methodology must have a sound physical basis according to current understanding. Other significant areas of uncertainty remain, for example knowledge of the stability functions (De Bruin et al., 1993; Hoedjes et al., 2002; Moene et al., 2004;

Meijninger et al., 2006) and accurate rejection of absorption fluctuations represented by the imaginary part of the refractive index, particularly for millimetre wavelengths (Nieveen et al., 1998; Green et al., 2001; Meijninger et al., 2002; Van Kesteren, 2008; Evans, 2009). To refine and improve the technique further careful experimental comparisons are required.

This improved methodology, based on theoretical considerations, should be applied to ensure that obtained latent heat fluxes are as accurate as possible, meet the accepted definition of surface flux and are comparable with other methods, such as eddy covariance.

Acknowledgements

We would like to thank Wim Kohsiek for his valuable discussions and the reviewers for their suggestions to strengthen the paper. This work was partly funded by the Natural Environment Research Council, UK.

Appendix

In Table A1 the structure parameter coefficients for absolute humidity (Q), specific humidity (q) and mass mixing ratio (r) formulations are given. These were derived starting from (1), in each case substituting e/T as $R_v Q$, $R_v \rho q = R_v p q / RT$, or $R_v \rho_d r = R_v p r / (R_d + R_v r) T$, which are obtained combining the ideal gas law and Dalton's law of partial pressures. The terms are broadly arranged into columns pertaining to the differentiation process. The structure parameter coefficients A_Q , A_q and A_r are all similar as are the temperature structure parameter coefficients for optical wavelengths. The significant difference occurs between A_T and A_r or A_τ due to the third term, which is the differential of density with respect to temperature. A_r and A_τ are identical because neither q nor r is dependent on T .

It is valid to use any of the above pairs of structure parameters to partition C_n^2 into temperature and moisture fluctuations (via an equation of the form of (10)). Only q or r should be used with MOST. The latent heat flux can be found using q_* (17) or r_* :

$$L_v E = -\overline{\rho_d} L_v u_* r_* = -\overline{\rho} (1 - \overline{q}) L_v u_* r_* . \quad (A1)$$

Since both (17) and (A1) require a $(1-q)^{\pm 1}$ factor to find $L_v E$, there is no obvious preference for choosing r over q .

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Tables

Scalar, y	Mean, \bar{y}	Fluctuation, y'	Relative fluctuation, y'/\bar{y}	Optical		Millimetre	
				A_y	$A_y y'/\bar{y}$	A_y	$A_y y'/\bar{y}$
T [K]	288	1	3×10^{-3}	-2.70×10^{-4}	-9×10^{-7}	-4.13×10^{-4}	-1.4×10^{-6}
q [kg kg ⁻¹]	10^{-2}	10^{-4}	10^{-2}	-6.85×10^{-7}	-6.9×10^{-9}	7.14×10^{-5}	7.1×10^{-7}
p [Pa]	10^5	10^{-1}	10^{-6}	2.70×10^{-4}	2.7×10^{-10}	3.40×10^{-4}	3.4×10^{-10}

Table 1 Sensitivity of the refractive index at optical and millimetre wavelengths to fluctuations in T , q and p . Estimates of turbulent fluctuations of T , q and p are from Moene et al. (2004), with p' estimated as $\rho u'^2$ using $u' \approx 0.3 \text{ m s}^{-1}$. A_y values assume typical atmospheric conditions ($T = 288 \text{ K}$, $p = 10^5 \text{ Pa}$, $q = 0.010 \text{ kg kg}^{-1}$). A wavelength of $0.880 \mu\text{m}$ was used for the optical region.

	$A_t = -\frac{\bar{p}}{T} \left(b_{t1} + b_{t2} \frac{R_v}{R} \bar{q} \right)$	$A_q = \frac{\bar{p}}{T} \frac{R_v}{R} \bar{q} b_{q2} \left(1 - \frac{\bar{q}}{R} (R_v - R_d) \right)$
Optical	$b_{t1} = 10^{-6} m_{1_opt}$ $= \left(0.237134 + \frac{68.39397}{130 - \lambda^{-2}} + \frac{0.45473}{38.9 - \lambda^{-2}} \right) \times 10^{-6}$ $b_{t2} = 10^{-6} (m_{2_opt} - m_{1_opt})$ $= (0.648731 + 0.0058058\lambda^{-2} - 0.000071150\lambda^{-4}$ $+ 0.000008851\lambda^{-6}) \times 10^{-6} - b_{t1}$	$b_{q2} = b_{t2}$
Millimetre-wave	$b_{t1} = 10^{-6} m_{1_mw}$ $= 0.776 \times 10^{-6}$ $b_{t2} = 10^{-6} m_{2_mw} + 10^{-6} (m_{2_mw} - m_{1_mw})$ $= \left(\frac{7500}{T} - 0.056 \right) \times 10^{-6}$	$b_{q2} = 10^{-6} (m_{2_mw} - m_{1_mw})$ $= \left(\frac{3750}{T} - 0.056 \right) \times 10^{-6}$

Table 2 Simplified forms of the temperature and humidity structure parameter coefficients for optical and millimetre wavelengths, in terms of specific humidity. Using this notation A_t and A_q have the same form for both wavelength regions, with the b -coefficients containing the wavelength (in μm) and temperature dependence. For optical regions b_{t1} , b_{t2} and b_{q2} depend on wavelength: for $\lambda_{opt} = 0.880 \mu\text{m}$, $b_{t1} = 0.781 \times 10^{-6} \text{ K Pa}^{-1}$ and $b_{t2} = b_{q2} = -0.124 \times 10^{-6} \text{ K Pa}^{-1}$ (to 3 significant figures); for millimetre wavelengths b_{t1} is constant, b_{t2} and b_{q2} depend on temperature.

Temperature Coefficients			
Optical	$A_{T_opt} = -10^{-6} m_{1_opt} \frac{\overline{p}}{\overline{T}}$		
	-271	-271	-
	$A_{t_opt} = -10^{-6} m_{1_opt} \frac{\overline{p}}{\overline{T}} - 10^{-6} (m_{2_opt} - m_{1_opt}) R_v \frac{\overline{pq}}{\overline{RT}}$		
	-270	-271	0.689
	$A_{r_opt} = -10^{-6} m_{1_opt} \frac{\overline{p}}{\overline{T}} - 10^{-6} (m_{2_opt} - m_{1_opt}) \frac{R_v \overline{pr}}{\overline{T(R_d + R_v r)}}$		
	-270	-271	0.689
Millimetre-wave	$A_{T_mw} = -10^{-6} m_{1_mw} \frac{\overline{p}}{\overline{T}} - 10^{-6} m_{2b_mw} R_v \overline{Q}$		
	-342	-269	-72.1
	$A_{t_mw} = -10^{-6} m_{1_mw} \frac{\overline{p}}{\overline{T}} - 10^{-6} m_{2b_mw} \frac{R_v \overline{pq}}{\overline{RT}} - 10^{-6} (m_{2_mw} - m_{1_mw}) \frac{R_v \overline{pq}}{\overline{RT}}$		
	-413	-269	-72.1
	$A_{r_mw} = -10^{-6} m_{1_mw} \frac{\overline{p}}{\overline{T}} - 10^{-6} m_{2b_mw} \frac{R_v \overline{pr}}{\overline{T(R_d + R_v r)}} - 10^{-6} (m_{2_mw} - m_{1_mw}) \frac{R_v \overline{pr}}{\overline{T(R_d + R_v r)}}$		
	-413	-269	-72.1
Humidity Coefficients			
Optical	$A_{Q_opt} = 10^{-6} (m_{2_opt} - m_{1_opt}) R_v \overline{Q}$		
	-0.689	-0.689	-
	$A_{q_opt} = 10^{-6} (m_{2_opt} - m_{1_opt}) \frac{R_v \overline{pq}}{\overline{RT}} - 10^{-6} (m_{2_opt} - m_{1_opt}) \frac{R_v \overline{pq}}{\overline{RT}} \left[\frac{\overline{q}}{\overline{R}} (R_v - R_d) \right]$		
	-0.685	-0.689	0.00416
	$A_{r_opt} = 10^{-6} (m_{2_opt} - m_{1_opt}) \frac{R_v \overline{pr}}{\overline{T(R_d + R_v r)}} - 10^{-6} (m_{2_opt} - m_{1_opt}) \frac{R_v \overline{pr}}{\overline{T(R_d + R_v r)}} \left[\frac{\overline{q}}{\overline{R}} R_v \right]$		
	-0.678	-0.689	0.110
Millimetre-wave	$A_{Q_mw} = 10^{-6} (m_{2_mw} - m_{1_mw}) R_v \overline{Q}$		
	71.8	71.8	-
	$A_{q_mw} = 10^{-6} (m_{2_mw} - m_{1_mw}) \frac{R_v \overline{pq}}{\overline{RT}} - 10^{-6} (m_{2_mw} - m_{1_mw}) \frac{R_v \overline{pq}}{\overline{RT}} \left[\frac{\overline{q}}{\overline{R}} (R_v - R_d) \right]$		
	71.4	71.8	-0.433
	$A_{r_mw} = 10^{-6} (m_{2_mw} - m_{1_mw}) \frac{R_v \overline{pr}}{\overline{T(R_d + R_v r)}} - 10^{-6} (m_{2_mw} - m_{1_mw}) \frac{R_v \overline{pr}}{\overline{T(R_d + R_v r)}} \left[\frac{\overline{q}}{\overline{R}} R_v \right]$		
	70.7	71.8	-1.15

Table A1 Structure parameter coefficients for optical and millimetre wavelengths for absolute humidity (A_T , A_Q), specific humidity (A_t , A_q) and mass mixing ratio (A_r , A_r) formulations. New formulations shown here are optical A_r and A_r and millimetre-wave A_t and A_q , and A_r and A_r . Values are shown for typical atmospheric conditions ($T = 288$ K, $p = 10^5$ Pa, $Q = 0.012$ kg m⁻³) below each term, including the total value of each structure parameter coefficient (shaded) to three significant figures. The values shown are scaled by a factor of 10^6 , so that e.g. $A_{t_mw} = -4.13 \times 10^{-4}$. A wavelength of 0.880 μ m was used for the optical region. The additional term appearing in A_t and A_r is significant (bold type), contributing around an extra 20% to the total structure parameter coefficients.

Figures

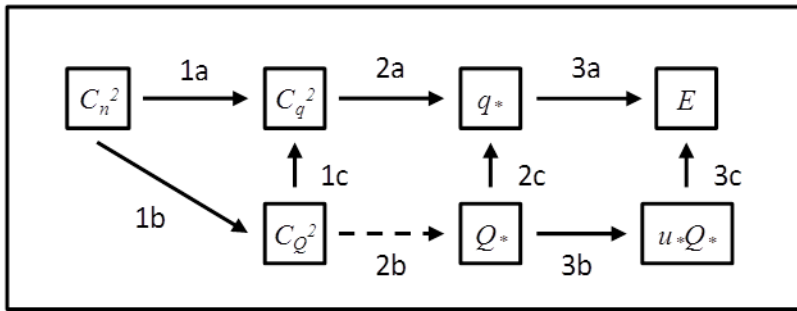


Figure 1 Summary of processing routes for absolute (Q) and specific (q) humidity formulations: 1. Partitioning of refractive index fluctuations into temperature and moisture fluctuations; 2. MOST; 3. Definition of evaporation (Eq 17). Stage 2b is invalid as Q is not a conserved variable. Conversions from absolute to specific humidity variables can be performed at stage 1c (Eq 14), 2c or 3c (Eq 18). See text for further explanation.

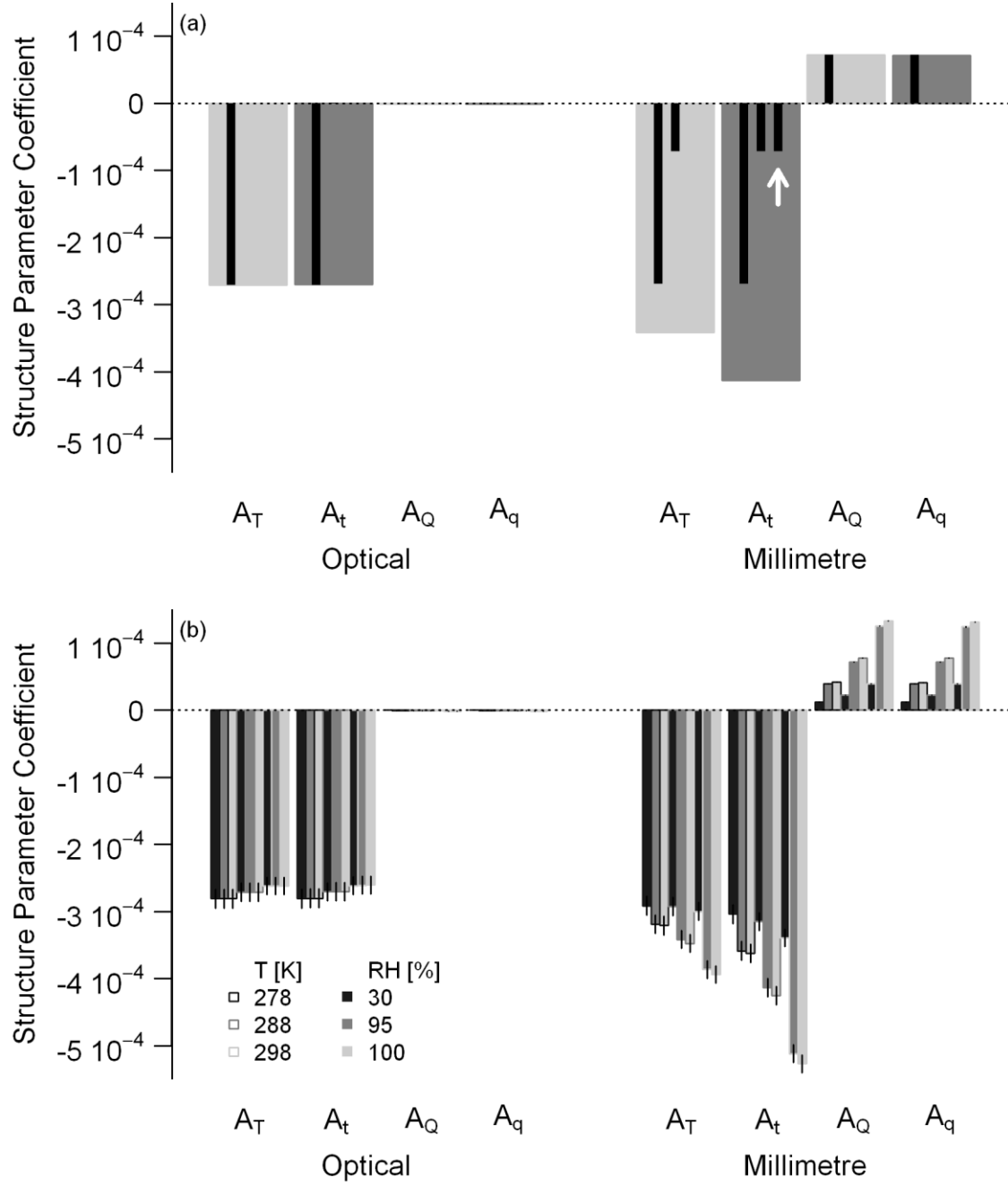


Figure 2 (a) Comparison of structure parameter coefficients (shaded bars) and contributions from each term in Table A1 (black) for typical atmospheric conditions (*viz.* $T = 288$ K, $p = 10^5$ Pa, $Q = 0.012$ kg m $^{-3}$, after Meijninger (2003)) for optical and millimetre wavelengths using absolute and specific formulations. The difference in millimetre wave A_t and A_T is caused by the differential of n_{v_mw} with respect to T appearing twice in A_t (arrow) and only once in A_T . The difference in optical A_Q and A_q is negligible (see Appendix). **(b)** Variation of the structure parameter coefficients for different temperatures and relative humidities (values in key). The central bar in each group ($T = 288$ K, $Q = 0.012$ kg m $^{-3}$) is equivalent to (a). Impact of pressure variations of $\pm 5 \times 10^3$ Pa are shown by the thin vertical lines.

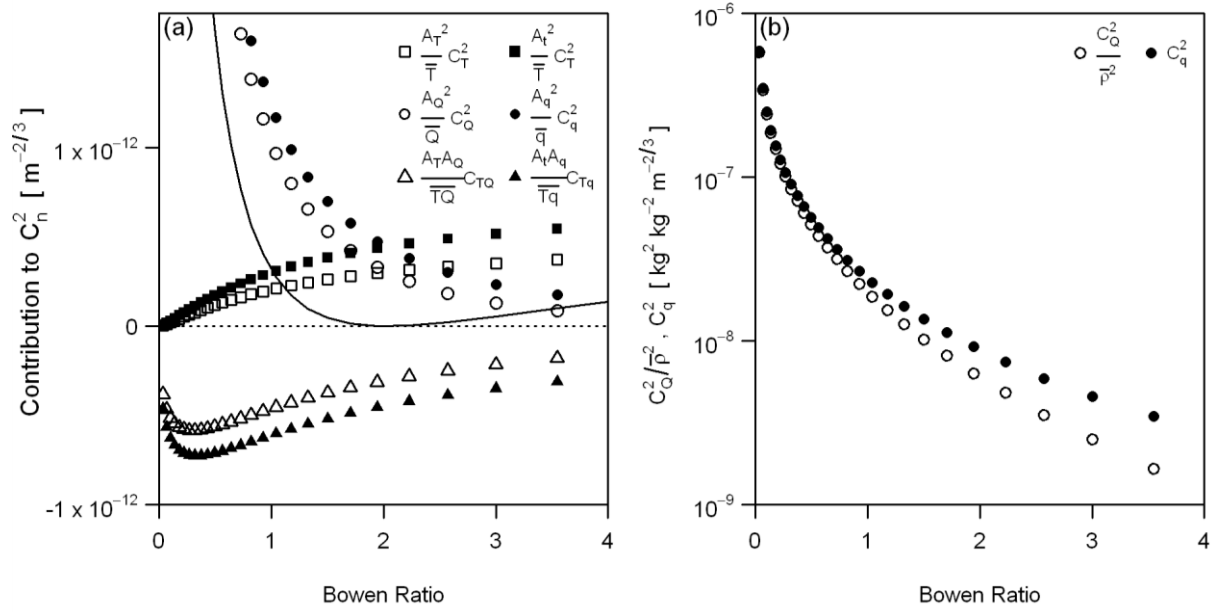


Figure 3 (a) Contribution of temperature, humidity and temperature-humidity fluctuations to the total C_n^2 (solid line) for millimetre wavelengths for the absolute and specific humidity methods, and (b) comparison between humidity structure parameters for a range of Bowen ratios with an available energy of 500 W m^{-2} , assuming the free convection limit and typical atmospheric conditions ($T = 288 \text{ K}$, $p = 10^5 \text{ Pa}$, $Q = 0.012 \text{ kg m}^{-3}$).

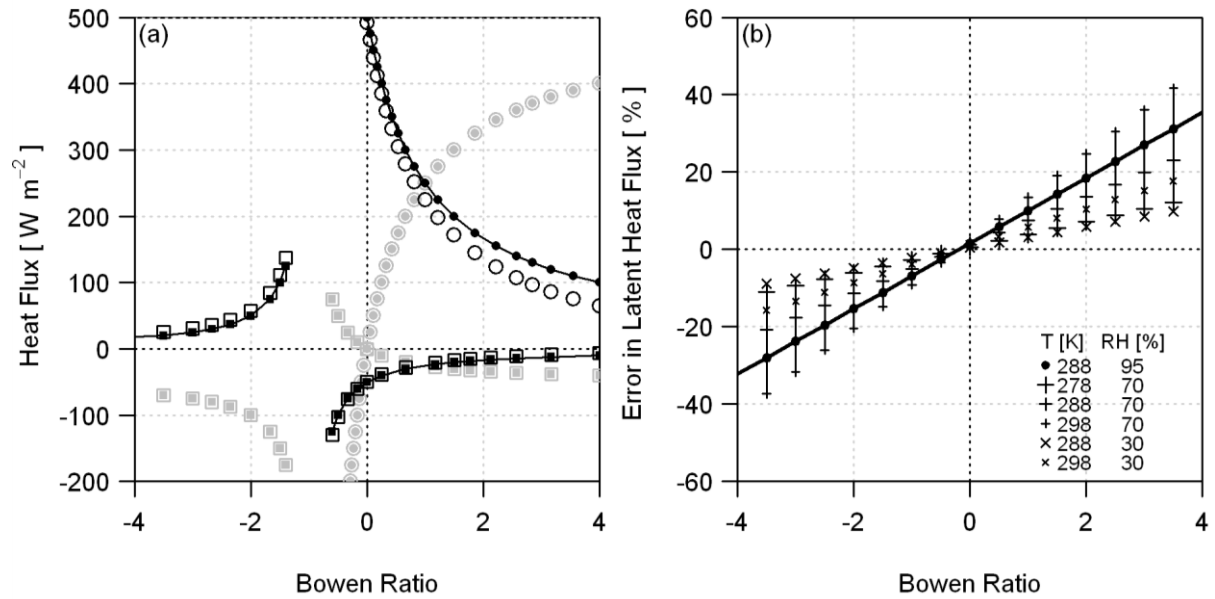


Figure 4 (a) Turbulent sensible (grey) and latent (black) heat fluxes as a function of Bowen ratio using absolute (hollow) and specific (filled) humidity formulations. Results when the available energy is 500 W m^{-2} (circles) and -50 W m^{-2} (squares) are shown and $T = 288 \text{ K}$, $p = 10^5 \text{ Pa}$, $Q = 0.012 \text{ kg m}^{-3}$. Sensible heat flux is unaffected by the choice of humidity whereas $L_v E$ via the absolute formulation ($-L_v u_* Q_*$) underestimates the magnitude of the true latent heat flux (17) for $\beta > 0$ and overestimates it for $\beta < 0$. (b) Percentage error in latent heat flux: $[(1 - (-L_v u_* Q_*)) / L_v E]$ according to (17) as a function of Bowen ratio, determined for typical T , p and Q as in (a) (solid line, solid circles) with vertical lines illustrating the effect of different atmospheric conditions (key).