Calculating and converting between common water vapour measures in meteorological data and their use in support of earth observation validation

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Foreword

During field missions associated with remote sensing calibration and validation as well as in processing (especially atmospheric correction) and applications undertaken by many scientists in the CSIRO Earth Observation Centre (EOC) there are many occasions when measures of water vapour are important and also need to be calculated or converted between different expressions. The set of formulae collected together in this report have arisen from two sources; one was the work done in CSIRO Water Resources between 1989 and 1994 when airborne and space based (AVHRR) thermal and visible region data were being used to estimate the spatial distribution of energy balance components and the other was in the ancillary data analyses associated with field missions in support of airborne and space based spectral sensing. The second has been a special focus of the CSIRO EOC in recent years with missions in support of airborne HyMap and space borne Hyperion hyperspectral data. In all this time – and even now with so much readily available via the web, it has often been difficult to conveniently find the full set of formulae such as have been provided in this report. Its first aim has therefore been to carefully collate and set out convenient and useful formulae and enable people to use them in their work. Its secondary aim has been to describe a typical application in which many of these formulae are needed for the development of ancillary data and analysis of the environmental situation in which the work has been carried out. Since units and errors are important aspects of any work with measurements – whether of water vapour or anything else – they are discussed as well in appendices. It is hoped that this report will be useful to the “EO Crew” that has been involved in the many missions of the past three years and also to others in the future.

David L B Jupp
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1 Introduction

Meteorological environmental data, in particular the vertical and temporal variations of water vapour in the atmosphere obtained from different instruments or data presentations, are often represented in one of a number of different but equivalent ways. In most cases, the data must be converted to other measures for use in environmental or atmospheric models. In particular, this has occurred in the CSIRO Earth Observation Centre (EOC) and Divisional field experiments that have been pursued in support of earth observation and remote sensing. These experiments involved the use of weather stations, radiosondes, sun photometers, irradiance data and other instruments, as well as ancillary data describing the local or regional meteorology and climate collected by other groups – such as the Australian Bureau of Meteorology (ABoM). In most cases, the water vapour information from these sources must be converted to other forms to reach the conclusions needed for the experiments.

In some of these situations, a primary output has been the column water vapour, or precipitable water in the atmosphere, and possibly some measure of the vertical distribution of water vapour density. This information can be used (for example) to validate surface measurements using radiative transfer calculations. Water vapour is a major absorbing material with spectrally distinct effects and its vertical distribution governs how its behaviour interacts with other absorbing and/or scattering materials present in the atmospheric column. Sometimes the water vapour in the atmosphere (or “aloft” as described in Reitan, 1963) is estimated from surface observations or in other cases more directly from radiosondes. In different situations again, such as where remotely sensed surface temperature is used to estimate evapotranspiration, there is a need to express water vapour as vapour pressure or to compute the saturated vapour pressure deficit. In these and other cases there is a need to flexibly transform between different measures of the amount of water vapour in the atmosphere.

In this Report, it is assumed that air (or dry-bulb) temperature \( T_a \) [°C] is always measured and that pressure \( P \) [kPa]\(^1\) (or an effective estimate of it) is available at the levels where the data relating to water vapour content of the atmosphere are taken. The water vapour information is measured in addition to these basic data and may take a number of forms in the data and be needed in various other forms in the analysis. The main ways in which water vapour amounts in the air have been recorded or provided from local surface observations, weather stations and radiosonde data obtained for the CSIRO EOC projects or in published regional climate Tables such as Maher and Lee (1977) have been:

- Mass mixing ratio \( m_r \) [g kg\(^{-1}\)];
- Relative humidity \( RH \) expressed as a percent [%];
- Dew-point temperature \( T_d \) [°C]; and
- Wet-bulb temperature \( T_w \) [°C].

\(^1\) Note: 1 kPa or kilo-Pascal is 10 mb or millibars. Hence 1000 mb is 100 kPa or 1000 hPa (hecto-Pascal). Units are discussed more generally in Appendix 1. Wherever possible, but respecting conventions as discussed in Appendix 1, SI units are used in this Report.
From any one these we often wish to compute one or all of:

- Density of water vapour \( (\rho_w) \) \([g \, m^{-3}]\);
- Vapour pressure \( (e_a) \) \([kPa]\); and
- Vapour pressure deficit \( (VPD) \) \([kPa]\).

In addition to computing these three outputs, it is often useful to compute the other possible inputs from the one given in the input data set. Providing simple equations to do this in spreadsheets, macros or programs is the objective of this document. Some other, less common, measures of water vapour (such as mole ratio and number density) bear simple relationships to the above and are also discussed in Appendix 1.

The basic definitions, approximations and fundamental constants we will use to convert between these quantities have been selected for convenience and ease of use by a wide range of people for a variety of practical purposes. In some cases (which will be noted) more accurate methods exist which can be used if the data quality and purposes of the analysis warrant. The level of accuracy and practicality has been taken to be similar to that outlined in Smith et al. (1992) and its revision by Allen et al. (1998), which are aimed primarily at the needs of agrometeorology and estimating evapotranspiration. However, the selected formulae have also been applied to upper air data and seem sufficiently accurate for the purposes for which they were collected when checked against outputs from the computer programs that are provided by Beer (1990).

The report starts with a discussion of the basic formulae on which the expressions are based. These are derived primarily in terms of the gas law and other principles of "ideal" gases. We then proceed to list the conversions in a convenient set of equations with example calculations and finally discuss a field experiment where many of the conversions were used to analyse the atmospheric water vapour for the purposes of remote sensing validation.

2 The Gas Law and basic expressions for water vapour amount

2.1 Density of Water Vapour

Water vapour density \( (\rho_w) \) with units \([g \, m^{-3}]\) is the mass of water vapour per unit volume of moist air. It has also been called the "absolute humidity" or "vapour concentration".

From the basic gas law (as outlined, for example, by Monteith and Unsworth, 1990 Chapter 2 or Harrison, 1963a) for an ideal gas:

\[
P V_m = R T_x
\]

where:
\[ P \] is the pressure of the gas \([kPa]\)
\[ V_m \] is the molar volume (volume occupied by a mole weight of gas for the given conditions) \( [m^3\, mol^{-1}] \)
\[ R \] is the universal gas constant \((8.31432) \,[kJ\,K^{-1}\,mol^{-1}]\) and
\[ T_K \] is the gas temperature in Kelvin \([K]\)

The molar volume of a gas is the volume with mass equal to the molecular weight. Hence, the density \((\rho)\) of the gas can be written as the ratio of its molecular weight divided by its molar volume in terms of the gas law as follows:

\[
\rho = \frac{M}{V_m} = \frac{PM}{RT_K}
\]

where, in addition to the previously defined terms:

\[ M \] is the molecular weight \([g\, mol^{-1}]\)

It follows that water vapour density \((\rho_w)\) or absolute humidity (Monteith and Unsworth, 1990; Harrison, 1963) with units \([g\, m^{-3}]\) can be written as:

\[
\rho_w = \frac{M_w}{V_a} = \frac{M_w e_a}{RT_K} = 2166.79 \frac{e_a}{(T_a + T_o)}
\]

where:

\[ M_w \] is the molecular weight of water \((18.01534)^2\) \([g\, mol^{-1}]\)
\[ V_a \] is the molar volume of air \([m^3\, mol^{-1}]\)
\[ e_a \] is the vapour pressure \([kPa]\)
\[ R \] is the universal gas constant \((8.31432) \,[J\,K^{-1}\,mol^{-1}]\)
\[ T_K \] is air temperature in Kelvin \([K]\)
\[ T_a \] is air temperature in degrees centigrade \([^\circ C]\)
\[ T_0 \] is the ice point for pure water at 1 atmosphere pressure \((101.325) \,[kPa]\) in absolute temperature \((273.15) \,[K]\)

\(^2\) Molecular weight is on the C\(_{12}\) scale and gases assumed ideal as outlined in Harrison (1963).
In the above equation, the ratio of \( M_w \) to \( R (2.16679) \) is multiplied by 1000 to bring the units of water vapour density to \([g\,m^{-3}]\). The gas law thereby provides a simple relation between water vapour density (or absolute humidity) and the vapour pressure.

### 2.2 Mass mixing ratio

The mass mixing ratio \((m_r)\) expressed as \([g\,kg^{-1}]\) is the mass of water vapour (as grams) per unit mass of dry air (as kilograms).

\[
m_r = 1000 \times \frac{\rho_w}{\rho_d}
\]

where:

- \(\rho_w\) the density of water vapour \([g\,m^{-3}]\) and
- \(\rho_d\) is the density of dry air \([g\,m^{-3}]\).

The density of dry air (in units of \([g\,m^{-3}]\)) is also found using the gas law by noting that the pressure of dry air is the total pressure minus the vapour pressure. This difference is then divided by the gas constant and the absolute temperature to yield:

\[
\rho_d = \frac{M_A(P - e_a)}{R T_k} = \frac{M_A(P - e_a)}{R (T_a + T_0)}
\]

where in addition to previously defined terms:

- \(M_A\) is the molecular weight of air (28.945) \([g\,mol^{-1}]\)

From this and the previous expression for \(\rho_w\) it follows that the mixing ratio \((m_r)\) \([g\,kg^{-1}]\) is:

\[
m_r = 1000 \times \frac{\rho_w}{\rho_d} = 1000 \times \frac{\epsilon}{\rho_d} \frac{e_a}{P - e_a} \approx 621.98 \frac{e_a}{P - e_a} \tag{4}
\]

The dimensionless constant \(\epsilon = 0.62198\) is the ratio of the relative molar masses of water and dry air \((M_w/M_A\)). It is multiplied here by 1000 to bring the result to the conventional units of mixing ratio of \([g\,kg^{-1}]\).
Inversely, if \( m_r \) is given we can write:

\[
e_a = \frac{m_r P}{621.98 + m_r}.
\] (5)

The gas law therefore also provides a simple relationship between mixing ratio, vapour pressure and atmospheric pressure (which we have assumed has been measured or estimated).

### 2.3 Relative humidity and saturation

The relative humidity (\( RH \) [\%]) is defined as (Monteith and Unsworth, 1990) the ratio of vapour pressure to saturated vapour pressure at the air temperature (\( T_a \)) expressed as a percent:

\[
RH = 100 \times \frac{e_a}{e^*(T_a)}
\] (6)

where:

- \( e^*(T) \) [kPa] is the saturated vapour pressure for moist air at temperature \( T \) [°C].

The definition and computation of “saturation” involves consideration of equilibrium and changes of phase as outlined by Harrison (1963a). In the projects that this document is designed to serve, the form of saturation that is most relevant is that of moist air with respect to liquid water.

While saturation will be treated simply here its strict definition is not simple since to quote from Harrison (1963a):

“Moist air at a given pressure and temperature is said to be saturated with respect to liquid water if its mixing ratio (or mole fraction of water vapour) is such that the moist air under these conditions can coexist in neutral equilibrium with clean liquid water at the same temperature and subjected to the same pressure, when the surface of separation between the phases is plane.”

To compute the saturated vapour pressure values in the practical situations covered in this report we have used the following approximation (Tetens, 1930; as expressed by Murray, 1967):

\[
e^* = 0.61078 \times e^{\frac{17.269 T_a}{T_a + 237.39}}.
\] (7)
The Tetens formula\(^3\) and its derivative are widely used in agro-meteorology (Smith \textit{et al}., 1992; Allen \textit{et al}., 1998). A more precise method is the Goff-Gratch formula (Goff & Gratch, 1946; Murray, 1967). Murray (1967) provides convenient expressions for both the Goff-Gratch and Tetens formulae for saturation vapour pressure of moist air relative to planar surfaces of both water and ice. However, as shown by Murray (1967), little difference is observed in the outputs of these formulae over normal ranges of surface environmental parameters. Therefore, since the Tetens formula is invertible \((T_a \text{ can be easily derived from } e^*)\), it is more convenient to use in most cases.

Another water vapour measure that we will compute and has direct applications in evapotranspiration studies (eg see Garratt, 1992) is the difference between the saturated vapour pressure and the measured vapour pressure. It is called the “vapour pressure deficit” \([D \text{ [k Pa]}]:\)

\[ D = e^* (T_a) - e_a \]

We can also use the following (equivalent) expression for \(RH\):

\[ RH = \frac{100 \times \rho_w}{\rho_w^* (T_a)} \]

where:

\[ \rho_w^*(T) \text{ [g m}^{-3}\text{]} \text{ is the saturated density of water vapour at temperature } T \text{ [°C].} \]

The saturated water vapour density can be approximated by the empirical expression:

\[ \rho_w^* = A e^{a_0 + a_1 T_a + a_2 T_0} \quad (A = T_0 / (T_a + T_0)) \]

where:

\[ a_0 = 18.9766 \]
\[ a_1 = -14.9595 \]
\[ a_2 = -2.43882 \]

However, this expression is not invertible and is normally only used as a convenient way to derive \(\rho_w^*\) when this is of direct interest.

These formulae are accurate within the normal working range of temperature, pressure and humidity encountered in agrometeorology and agree well with alternative formulae when applied to atmospheric vertical profile data. In most cases,

\(^3\) The number 237.29 (or \(T = -35.86\)) in the Tetens formula is written for temperature in °C and is not the ice point \((T_0)\) written incorrectly!
there is more variation due to the lack of adherence to the conditions of the definition than there is between approximations.

### 2.4 Dew point temperature

The dew point temperature \((T_d)\) with units \([°C]\) is the temperature at which the air becomes saturated. That is (Monteith and Unsworth, 1990):

\[
e_a = e^*(T_d)
\]  

\(T_d [°C]\) can be obtained from \(e_a [kPa]\) using the Tetens approximation for the saturated vapour pressure in its convenient inverse form.

With “\(ln\)” representing Naperian logarithm (or base \(e\)), if we wish to compute \(T_d\) accurately in two steps (with intermediate calculation “\(H\)”) we could write:

\[
H = \frac{1}{17.269} \ln \left( \frac{e_a}{0.61078} \right)
\]

\[
T_d = \frac{237.29 \times H}{1 - H}
\]

Alternatively, we could use the direct (but slightly less precise) calculation:

\[
T_d = \frac{13.741 \times ln(e_a) + 6.7745}{0.97145 - 0.057907 \times ln(e_a)}
\]

\[= e^{*-1}(e_a)\]  

If \(T_d\) is given, \(e_a\) can be obtained directly using the Tetens formula and hence the other measures can be derived directly from \(e_a\).

### 2.5 Wet-bulb temperature

Wet-bulb temperature has been the most common method for obtaining water vapour information in traditional meteorological stations. As well as a measurement of (dry-bulb) air temperature, the temperature measured by an identical thermometer wrapped in a wet wick is measured as the “wet-bulb” temperature. It has also been the basis of measurements for more sophisticated techniques such as the Bowen Ratio.

The result is a quantity that can be used to compute all of the other quantities but which is a little more difficult to derive when one of the others is given. Detailed discussions of the physics behind the wet-bulb temperature and the associated psychrometer equation can be found in Monteith and Unsworth (1990), Harrison (1963b) or Brunt (1952, Sections 51-58).

The psychrometer equation has the form:
\[ e_a = e^*(T_w) - \gamma (T_a - T_w) \]

where

\[ \gamma \text{[kPa °C}^{-1}] \text{ is the psychrometric constant} \]
\[ T_w \text{ is the wet-bulb temperature [°C] and} \]
\[ T_a \text{ is dry-bulb (air) temperature [°C].} \]

For a ventilated system (Monteith and Unsworth, 1990; Harrison, 1963b):

\[ \gamma = \frac{C_p P}{\varepsilon \lambda} \]
\[ = 0.0016287 \frac{P}{\lambda} \]
\[ \approx 0.0667 \]  

where:

- \( C_p \) is the specific heat of moist air (1.013 x 10^{-3} [MJ kg^{-1} °C^{-1}])
- \( \varepsilon = 0.62198 \) is the [dimensionless] ratio of the relative molar masses of water and dry air
- \( P \) is the pressure [kPa]
- \( \lambda \) is the latent heat of vaporisation [MJ kg^{-1}].

A useful expression for \( \lambda \) (which varies slowly with temperature) is (using an empirical approximation given by Harrison, 1963b which is most accurate in the range 0 to 30 °C):

\[ \lambda(T) = 2.501 - 2.361 \times 10^{-3} T \cdot \]  

In this expression, \( T \) is °C. That is, if \( T_w \) is measured, the above expressions allow \( e_a \) to be determined and hence the others as described below.

If \( e_a \) and \( T_a \) are known then \( T_w \) can be found by a method of nonlinear iteration to find the solution of the equation,

\[ f(T_w) = e_a - e^*(T_w) + \gamma (T_a - T_w) = 0. \]

Alternatively, expanding the saturated vapour function about \( T_a \) provides the following first order approximation using the vapour pressure deficit \( (D) \) that may be used if accuracy in the wet-bulb temperature estimate is not critical and humidity is not at the dry end (e.g. \( RH > 30\% \)):
Here $\Delta [kPa \, ^\circ C^{-1}]$ is the slope of the saturation vapour pressure relationship at $T_a$:

$$\Delta = \frac{\partial e^*(T)}{\partial T}_{T_a}$$

$$\approx \frac{4097.76 \, e^*(T_a)}{(T_a + 237.29)^2} \quad (12)$$

Methods for solving the expression for $T_w$ more accurately are further discussed in Appendix 2. In general, $T_w$ is not of great interest as a conversion from other measures of water vapour. Its main interest occurs when it is the measured quantity and the (simpler) task is to convert it to another measure.

### 2.6 Accuracy of the calculated measures

When the water vapour measures are derived from input data the level of accuracy of the input data inevitably leads to a level of accuracy in the derived expressions that it is usually very valuable to know. At very least it allows you to choose how many significant places to include in the results.

In the following sections, we will provide some values for the “precision” of the results based on the following approach. The input data will always be air temperature ($T_a$), air pressure ($P$) and one of a number of measures of the water vapour ($I_w$). If we have some knowledge of the variability of these inputs they will be expressed in terms of standard deviations of the form $\pm \sigma(T_a), \pm \sigma(P)$ and $\pm \sigma(I_w)$. At very least these will be the range that will not change the input value to the number of significant figures in which it was provided. For example, a value of $T_a$ as 23.4 °C can be given a standard deviation of $\sigma(T_a) = \pm 0.04$.

In all cases, the output water vapour measure ($O_w$) is a function of one, two or all three of these inputs. The corresponding standard deviation for the output value can be approximated as:

$$\sigma(O_w) = \left( \left[ \frac{\partial O_w}{\partial T_a} \right]^2 \sigma^2(T_a) + \left[ \frac{\partial O_w}{\partial P} \right]^2 \sigma^2(P) + \left[ \frac{\partial O_w}{\partial I_w} \right]^2 \sigma^2(I_w) \right)^{1/2}.$$  

This is a conservative estimate based on the assumption that the variations are independent. Since the partial derivatives are a little complex they have been collected in tables in Appendix 3. They have been used in the examples and are straightforward, if tedious, to add to a spreadsheet for the outputs derived here. It is up to the user of the formulae whether this is implemented or not – but it is useful to do it.
3 Converting between expressions

The above expressions can be used to convert between the various forms when pressure \( P \) [kPa] and temperature \( T_a \) [°C] plus one of the forms are known. However, if the pressure \( P \) [kPa] at a site is not known there will be some error if the mixing ratio is involved. In this case pressure could be estimated from the altitude above sea level (ASL) using a locally developed expression (that may depend on time of year) or some default such as the following (based on the annual mean for the 10 year record between 1965 and 1975 at Wagga in central NSW as listed in Maher and Lee, 1977):

\[
P(z_0) = P_0 e^{-z_0(d_0+a_tz_0)}
\]
\[
P_0 = P(0) = 101.325
\]
\[
d_0 = 1.198 \times 10^{-4}
\]
\[
a_t = 1.26 \times 10^{-9}.
\]

In this expression, \( P_0 \) is in kPa (not hPa or mb) and \( z_0 \) is in metres (not km) ASL. However, wherever possible, local pressure should be measured with a well-maintained weather station when used for remote sensing calibration and validation.

In the case where pressure is only known at a location away from the site at an altitude \( z_1 \) ASL, the above (or similar) equation can be used to scale the pressure based on the height difference (\( \delta z \)) to obtain the local value of \( P_0 \):

\[
P(z_1) = P(z_0) e^{-\delta z(d_0+a_t(z_1+z_0))}
\]
\[
\delta z = z_1 - z_0
\]

The resulting equation could be used to estimate \( P \) at any altitude (\( z \) metres ASL) using the adjusted value of \( P_0 \).

The lists of expressions on the following pages allow direct entry of the relevant equations into a spreadsheet, macro or procedure. They assume only that the expressions for saturated vapour pressure and its derivative (\( e^*(T) \), Eq 7 and \( \Delta \), Eq 12) and that for gamma (\( \gamma \), Eq 10), which depend only on air temperature and pressure, have been computed as:

\[
e^* = 0.61078 \times e^{\frac{17.269 \times T_u}{T_u + 237.29}}
\]
\[
\Delta = \frac{4097.76 \times e^*(T_u)}{(T_u + 237.29)^2}
\]
\[
\gamma = \frac{1.6287 \times 10^{-3} \times P}{2.501 - 2.361 \times 10^{-3} \times T_u}.
\]
3.1 Case 1: Mixing ratio ($m_r$) given

The (mass) mixing ratio $m_r$ [g kg$^{-1}$] is used in Maher and Lee (1977) for the long term averages of atmospheric water vapour. Due to the variability of water vapour it is a median value for the 10 years.

It follows from the above that for $P$ in [kPa] and $m_r$ in [g kg$^{-1}$]:

$$e_a = \frac{m_rP}{621.98 + m_r}.$$  

Hence:

$$\rho_w = 2166.8 \frac{e_a}{(T_a + T_o)}$$

$$RH = 100 \times \frac{e_a}{e^*(T_a)}$$

$$D = e^*(T_a) - e_a$$

$$T_a = e^{-t_e}(e_a) = \frac{13.741 \times \ln(e_a) + 6.7745}{0.97145 - 0.057907 \times \ln(e_a)}$$

$$T_w = T_a - \frac{D}{\Delta + \gamma}.$$ 

The starting calculations with $P$ and $T_o$ provided (input items are in **bold**) are:

<table>
<thead>
<tr>
<th>$P$ [kPa]</th>
<th>$T_o$ [°C]</th>
<th>$e^*(T_o)$ [kPa]</th>
<th>$\Delta$ [kPa °C$^{-1}$]</th>
<th>$\gamma$ [kPa °C$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>98.0</td>
<td>22.0</td>
<td>2.644</td>
<td>0.1611</td>
<td>0.0652</td>
</tr>
<tr>
<td>(0.02)</td>
<td>(0.02)</td>
<td>(0.003)</td>
<td>(0.0002)</td>
<td>(0.00001)</td>
</tr>
</tbody>
</table>

Using data from the Wagga meteorological station that will be described in the example but with “rounded” primary input for some realism:

<table>
<thead>
<tr>
<th>$m_r$ [g kg$^{-1}$]</th>
<th>$e_a$ [kPa]</th>
<th>$\rho_w$ [gm$^{-3}$]</th>
<th>RH [%]</th>
<th>$D$ [kPa]</th>
<th>$T_d$ [°C]</th>
<th>$T_w$ [°C]</th>
<th>$T_w$ (acc)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.7</td>
<td>0.580</td>
<td>4.26</td>
<td>21.92</td>
<td>2.064</td>
<td>-0.68</td>
<td>12.88</td>
<td>10.89</td>
</tr>
<tr>
<td>(0.02)</td>
<td>(0.003)</td>
<td>(0.03)</td>
<td>(0.12)</td>
<td>(0.004)</td>
<td>(0.07)</td>
<td>(0.01)</td>
<td>(0.01)</td>
</tr>
</tbody>
</table>

Since the situation was dry (RH < 30%) the difference between the approximate wet-bulb temperature and the iterated (“acc” for accurate) value obtained as described in Appendix 2 is significant at 2°C.

The numbers in (brackets) are the computed standard deviations described earlier and using the partial derivatives in Appendix 3. The assumed variation in the inputs is small here to illustrate the variations without losing too many places.
3.2 Case 2: Relative humidity (RH) given

If RH is the form in which the data are provided (as is common in processed daily radiosondes and weather station data such as those in the example) it follows that with $T_a$ in [ °C]:

$$e_a = \frac{RH \times e^*(T_a)}{100}.$$ 

Hence the other expressions can be obtained as:

$$\rho_w = 2166.8 \frac{e_a}{(T_a + T_b)}$$

$$D = e^*(T_a) - e_a$$

$$m_v = 621.98 \frac{e_a}{P - e_a}$$

$$T_d = e^{-1}(e_a) = \frac{13.741 \times \ln(e_a) + 6.7745}{0.97145 - 0.057907 \times \ln(e_a)}$$

$$T_w \approx T_a - \frac{D}{\Delta + \gamma}.$$ 

Again, the starting calculations are:

<table>
<thead>
<tr>
<th>$P$ [kPa]</th>
<th>$T_a$ [°C]</th>
<th>$e^*(T_a)$ [kPa]</th>
<th>$\Delta$ [kPa °C$^{-1}$]</th>
<th>$\gamma$ [kPa °C$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>98.0</td>
<td>22.0</td>
<td>2.644</td>
<td>0.1611</td>
<td>0.0652</td>
</tr>
<tr>
<td>(0.02)</td>
<td>(0.02)</td>
<td>(0.003)</td>
<td>(0.0002)</td>
<td>(0.00001)</td>
</tr>
</tbody>
</table>

If the relative humidity is used as the input for the Wagga data (as was provided in the actual case) we have:

<table>
<thead>
<tr>
<th>RH [%]</th>
<th>$e_a$ [kPa]</th>
<th>$\rho_w$ [gm$^{-3}$]</th>
<th>$D$ [kPa]</th>
<th>$m_v$ [g kg$^{-1}$]</th>
<th>$T_d$ [°C]</th>
<th>$T_w$ [°C]</th>
<th>$T_w$(acc)</th>
</tr>
</thead>
<tbody>
<tr>
<td>22.0</td>
<td>0.582</td>
<td>4.27</td>
<td>2.062</td>
<td>3.71</td>
<td>-0.63</td>
<td>12.89</td>
<td>10.91</td>
</tr>
<tr>
<td>(0.02)</td>
<td>(0.001)</td>
<td>(0.01)</td>
<td>(0.003)</td>
<td>(0.01)</td>
<td>(0.02)</td>
<td>(0.01)</td>
<td>(0.01)</td>
</tr>
</tbody>
</table>

In the example discussed later, readers may notice that the dew point temperature is not quite the same. In the example provided later, the two step calculation was used.

In common with others it seems that the calculation of dew point temperature requires most input accuracy.
3.3 Case 3: Dew point temperature \((T_d)\) given

Daily radiosonde data are often provided as dew point temperature rather than humidity and it is the measured data from a hygrometer. In other situations, when there are no water vapour data available, the average vapour density is sometimes estimated by assuming daily minimum temperature is at dew point (Dyer and Brown, 1977; Bristow, 1992). Again, dew point is used as a starting value. In such cases, with dew point temperature \((T_d)\) in \([\,^\circ C]\):

\[
e_a = e^*(T_d)
\]

and the other measures follow as described before:

\[
\rho_w = 2166.8 \frac{e_a}{(T_a + T_0)}
\]

\[
RH = 100 \times \frac{e_a}{e^*(T_a)}
\]

\[
D = e^*(T_a) - e_a
\]

\[
m_t = 621.98 \frac{e_a}{P - e_a}
\]

\[
T_w \approx T_a - \frac{D}{\Delta + \gamma}
\]

In the case of the daily minimum temperature being used to estimate average water vapour density or vapour pressure assuming it is the dew point (dew often occurs at minimum temperature), the water vapour pressure or density are sometimes assumed to be constant over the day to model the variation in (say) humidity. The variation is due to the changing role of temperature in the calculations.

Again, the starting calculations are:

<table>
<thead>
<tr>
<th>(P \text{ [kPa]})</th>
<th>(T_a \text{ [}^\circ C)</th>
<th>(e^*(T_a) \text{ [kPa]})</th>
<th>(\Delta \text{ [kPa} , ^\circ C^{-1})</th>
<th>(\gamma \text{ [kPa} , ^\circ C^{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>98.0</td>
<td>22.0</td>
<td>2.644</td>
<td>0.1611</td>
<td>0.0652</td>
</tr>
<tr>
<td>(0.02)</td>
<td>(0.02)</td>
<td>(0.003)</td>
<td>(0.0002)</td>
<td>(0.00001)</td>
</tr>
</tbody>
</table>

Using a rounded value of the dew point temperature from the Wagga data and following the list above the resulting data are:

<table>
<thead>
<tr>
<th>(T_d \text{ [}^\circ C)</th>
<th>(e_a \text{ [kPa]})</th>
<th>(\rho_w \text{ [g m}^{-3})</th>
<th>(RH \text{ [%]})</th>
<th>(D \text{ [kPa]})</th>
<th>(m_t \text{ [g kg}^{-1})</th>
<th>(T_w \text{ [}^\circ C)</th>
<th>(T_w (acc))</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.6</td>
<td>0.585</td>
<td>4.29</td>
<td>22.11</td>
<td>2.059</td>
<td>3.73</td>
<td>12.90</td>
<td>10.42</td>
</tr>
<tr>
<td>(0.02)</td>
<td>(0.001)</td>
<td>(0.01)</td>
<td>(0.04)</td>
<td>(0.003)</td>
<td>(0.01)</td>
<td>(0.01)</td>
<td>(0.01)</td>
</tr>
</tbody>
</table>

The dew point temperature is likely to be less accurate than was assumed so that in practice the derived measures may have an excessive precision.
3.4 Case 4: Wet-bulb temperature ($T_w$) given

Wet-bulb temperature often occurs in locally collected weather data – such as ancillary meteorological data collected on farms and stations where the data are simple, directly recorded from instruments and unprocessed. It is also the recorded quantity in some instruments used to measure Bowen Ratio.

In this case, with both dry-bulb ($T_a$) and wet-bulb ($T_w$) temperatures in [°C]:

$$e_a = e^*(T_w) + \gamma(T_w - T_a)$$

and the other expressions follow as described before:

$$\rho_a = 2166.8 \frac{e_a}{(T_a + T_d)}$$

$$RH = 100 \times \frac{e_a}{e^*(T_a)}$$

$$D = e^*(T_a) - e_a$$

$$m_r = 621.98 \frac{e_a}{P - e_a}$$

$$T_a = e^{-1}(e_a) = \frac{13.741 \times \ln(e_a) + 6.7745}{0.97145 - 0.057907 \times \ln(e_a)}.$$ 

Again, the starting calculations are:

<table>
<thead>
<tr>
<th>$P$ [kPa]</th>
<th>$T_a$ [°C]</th>
<th>$e^*(T_a)$ [kPa]</th>
<th>$\Delta$ [kPa °C⁻¹]</th>
<th>$\gamma$ [kPa °C⁻¹]</th>
</tr>
</thead>
<tbody>
<tr>
<td>98.0</td>
<td>22.0</td>
<td>2.644</td>
<td>0.1611</td>
<td>0.0652</td>
</tr>
<tr>
<td>(0.02)</td>
<td>(0.02)</td>
<td>(0.003)</td>
<td>(0.0002)</td>
<td>(0.00001)</td>
</tr>
</tbody>
</table>

Using the accurately iterated (see Appendix 2) wet-bulb temperature for the Wagga data – but rounded to a realistic value we find:

<table>
<thead>
<tr>
<th>$T_w$ [°C]</th>
<th>$e_a$ [kPa]</th>
<th>$\rho_a$ [gm⁻³]</th>
<th>$RH$ [%]</th>
<th>$D$ [kPa]</th>
<th>$m_r$ [g kg⁻¹]</th>
<th>$T_d$ [°C]</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.9</td>
<td>0.581</td>
<td>4.26</td>
<td>21.96</td>
<td>2.063</td>
<td>3.71</td>
<td>-0.66</td>
</tr>
<tr>
<td>(0.02)</td>
<td>(0.003)</td>
<td>(0.02)</td>
<td>(0.14)</td>
<td>(0.005)</td>
<td>(0.02)</td>
<td>(0.08)</td>
</tr>
</tbody>
</table>

It is more common for wet-bulb temperature to be an input than for it to be calculated as in previous cases.

The standard deviations again show how precision may be tracked if input accuracies – or simply precisions – are known or assumed.
4 An example of application for the formulae

4.1 Introduction

Among many possible uses of the formulae described in this Report it is appropriate to consider some of particular relevance to remote sensing missions for calibration and validation of satellite or airborne data.

The case we will discuss involved activities on January 12, 2002 when there was a conjunction of space, air and ground based data from a number of sensors and instruments for a site near Coleambally, NSW. The space data came from the EO-1 satellite (Hyperion and ALI sensors), the Landsat-7 satellite (ETM+ sensor), the SAC-C satellite and the TERRA satellite ASTER sensor (and potentially the MODIS sensor as well). The airborne data were HyMap scanner data flown by HyVista Corporation and a team from CSIRO collected and collated a range of ground data. Most of the remote sensing data collections were made near to 1000 Australian Eastern Standard Time (AEST), which is Coordinated Universal Time (UTC) plus 10 hours. Further information about the activity can be found in Datt et al. (2003).

Atmospheric water vapour affects many of the spectral regions of data collected by the instruments and knowing the amount and vertical distribution of water vapour is very useful for supporting corrections to the data and essential for calibration and validation experiments. With Hyperspectral instruments such as HyMap and Hyperion it is possible to develop estimates for total column water vapour (but not vertical distribution) from the data. However, for other instruments or to validate the estimates, it is very important to take appropriate data at the time of the ground activity.

Water vapour information at Coleambally was provided by:

- Radiosonde and surface data from an ABoM site at Wagga Wagga, NSW (150 km away);
- Surface meteorological data from a CSIRO automatic weather station system; and
- Total column water vapour estimates from a NASA AERONET CIMEL instrument.

The ABoM station at Wagga (to which Wagga Wagga is commonly abbreviated – and will be in the following) is Station number 90 at location 35.17 S 147.46 E and has altitude 213 metres ASL. There are also long term upper atmospheric data for Wagga (Maher and Lee, 1975) that can be used as a “climatological” base for estimating the water vapour data (amount and/or vertical distribution) in the absence of other information. This has also been used as an example for the calculations. Investigating the use of the local data (possibly in combination with the Wagga data) is especially important here as at 150 km distance, and due to its location in changing topographic conditions, the Wagga station is uncomfortably distant from the site at Coleambally. However, such distances to available data are not uncommon in Australia.
4.2 Atmospheric profile of water vapour

4.2.1 Basic Definitions

Data recorded at ABoM meteorological stations may include upper atmospheric information from radiosondes taken at selected times of the day. The base data sets they provide are the vertical profiles of pressure, air temperature and humidity (or some other measure of water vapour such as dew point temperature or mixing ratio) as a function of height above the ground. These data are fundamental to describing and the thermodynamics of the atmosphere as described in Iribarne and Godson (1973). For atmospheric modelling as it is used in correction of either visible and near infrared or thermal remote sensing data or for vicarious calibration studies, it is helpful to know about both the profile of water vapour and the total amount of water vapour in the atmospheric column. Both amount and profile are needed since the overall level of absorption in the water vapour bands is related to the total column water and the differential effects in different bands and interactions between water absorption and other effects (such as aerosol scattering) to the vertical distribution.

If the water vapour density at level $z$ ASL is denoted $\rho_w(z)$ then the total amount by mass of water vapour in the vertical column to space ($W$) can be written:

$$W = \int_{z_0}^{\infty} \rho_w(z) dz.$$ 

In this integral, $z_0$ is the altitude of the surface ASL. If the water vapour density is in $g\, m^{-3}$ as in this document, and the height is in $km$ the units of the integral will be $kg\, m^{-2}$, which is not a normally used unit although it is the SI unit. To obtain the more commonly used units for $W$ as $g\, cm^{-2}$ this value is multiplied by 10 (see Appendix 1). This same value is even more usually described in terms of an equivalent depth of liquid water as $cm$ of precipitable water. That is, it is the depth of liquid water that could conceptually be extracted from a column of area $1\, cm^2$ over the whole atmospheric column.

In addition, the absolute upper bound on the amount of precipitable water that can be supported can be calculated for the site and conditions as:

$$W^* = \int_{z_0}^{\infty} \rho_w^*(z) dz.$$ 

4.2.2 Scale height

Both the amount and profile of water vapour are variable on a short time scale but tend to have regional and seasonal characteristics. One way to summarise the vertical profile is in terms of the “scale height” ($H_w$) defined by:

$$H_w = \frac{\int_{z_0}^{\infty} \rho_w(z) dz}{\int_{z_0}^{\infty} \rho_w(z) e^{\frac{-z}{H_w}} dz}.$$
Clearly, as defined here, $W = H_w \rho_w(z_0)$, which defines the scale of the relationship between the surface level water vapour and the column water vapour. A default model for the profile that has the same total water vapour and surface value is that:

$$\rho_w(z) = \rho_w(z_0) e^{-\frac{(z-z_0)/H_w}{}}.$$

The persistence and long term validity of this simple model was proposed by Reitan (1963) and has been used by many authors – including Leckner (1978) for parameterising atmospheric radiation models. The default model can also provide a useful reference model against which to discuss vertical features such as moist or dry layers in the profile as will be seen below. It also provides a means to scale the column water into a restricted section of the profile as may be needed to compare results with those from an aircraft at height $h$ above the ground by scaling from the total column value to the column height to the aircraft:

$$W(z_0, h) = \int_{z_0}^{h} \rho_w(z)dz = H_w(z_0, h) \rho_w(z_0) \approx (1-e^{-\frac{(h-z_0)/H_w}{}})H_w\rho_w(z_0) = (1-e^{-\frac{(h-z_0)/H_w}{}})W.$$

The water vapour in radiosonde data is sometimes expressed as relative humidity (%) or dew point temperature and sometimes as mixing ratio. In all cases, combined with pressure and air temperature, the formulae described here allow the precipitable water and scale height to be computed.

### 4.2.3 Providing estimates for validation

Given these principles there are a number of ways that suggest themselves to obtain local and regional estimates of amount and vertical distribution of the water vapour. Some of these depend on the stability of the scale height or on a level of regional spatial dependency of the water vapour density. Each assumption has its limitations. However, among possible methods considered here are:

1. Using radiosonde data from a nearby meteorological station to obtain $W$ and $H_w$;
2. Using an estimate of the scale height $H_w$ to scale surface information to $W$; and
3. Using a sun photometer and surface information in combination to obtain $W$ and $H_w$.

While a complete study of these different methods and their value in remote sensing calibration and validation is beyond the scope of this Report, their use in this instance
provides a convenient example of different calculations we generally need to make to compare the various data sets.

4.3 Meteorological information from Wagga

4.3.1 Basic surface data at the ABoM station at Wagga

The weather at Coleambally and the nearby areas around the time of the mission was quite variable. Table 1 records surface observations at Wagga (which is 213 m ASL and 150 km from Coleambally) on the three days January 11, 12 and 13 close to the 1000 AEST conjunction of satellite, airborne and ground based data on January 12 (pressure given in hPa by the station and converted to kPa by dividing by 10):

<table>
<thead>
<tr>
<th></th>
<th>January 11</th>
<th>January 12</th>
<th>January 13</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure [kPa]</td>
<td>98.31</td>
<td>98.00</td>
<td>98.18</td>
</tr>
<tr>
<td>Air Temperature [°C]</td>
<td>24.6</td>
<td>22.0</td>
<td>17.3</td>
</tr>
<tr>
<td>Relative humidity [%]</td>
<td>39.0</td>
<td>22.0</td>
<td>30.0</td>
</tr>
<tr>
<td>Visibility [km]</td>
<td>4.0</td>
<td>30.0</td>
<td>30.0</td>
</tr>
</tbody>
</table>

The low visibility at Wagga on January 11 was caused by smoke from fires being brought in from the west. The EOC weather station data described in a following section showed the afternoon of January 11 to be hot and relatively humid with westerly winds and low visibility. It was most likely the same smoke that reduced the visibility in Wagga. A cold front from the south moved through during the night before the data collections, after which the visibility improved dramatically and the near surface air became much drier.

These data represent a conjunction of air temperature and humidity and from the Case 2 expressions above we arrive at the following results:

<table>
<thead>
<tr>
<th></th>
<th>January 11</th>
<th>January 12</th>
<th>January 13</th>
</tr>
</thead>
<tbody>
<tr>
<td>Saturated Vapour Pressure $e^* (T_v)$ [kPa]</td>
<td>3.093</td>
<td>2.644</td>
<td>1.975</td>
</tr>
<tr>
<td>Vapour Pressure $e_u$ [kPa]</td>
<td>1.206</td>
<td>0.582</td>
<td>0.592</td>
</tr>
<tr>
<td>Vapour Density $\rho_w$ [g $m^{-3}$]</td>
<td>8.78</td>
<td>4.27</td>
<td>4.42</td>
</tr>
<tr>
<td>Vapour Pressure Deficit $D$ [kPa]</td>
<td>1.887</td>
<td>2.062</td>
<td>1.382</td>
</tr>
<tr>
<td>Mixing ratio $m_\ell$ [g kg$^{-1}$]</td>
<td>7.73</td>
<td>3.71</td>
<td>3.78</td>
</tr>
<tr>
<td>Dew Point Temperature $T_d$ [°C]</td>
<td>9.73</td>
<td>-0.67</td>
<td>-0.42</td>
</tr>
<tr>
<td>Wet Bulb Temperature $T_w$ [°C]</td>
<td>17.06</td>
<td>12.89</td>
<td>10.02</td>
</tr>
</tbody>
</table>

The differences between the days are instructive. The dependence of relative humidity on air temperature can in some cases make relative humidity a misleading measure of
amount of water vapour\(^4\). The increase in relative humidity on January 13 to a similar value as it was on January 11 is mainly due to temperature effects since the water vapour amount on January 12 and 13 was about the same and much lower than it was on January 11. Vapour pressure, vapour density and mixing ratio tell a consistent story of a dry air mass replacing a moister air mass overnight between January 11 and 12.\(^5\)

### 4.3.2 Wagga daily radiosondes

Daily radiosondes were taken between 0930 and 1030 on the three days January 11, 12 and 13. The data provided by the ABOM record pressure, height, temperature, humidity and dew point temperature. Again it is straightforward to compute the terms needed and especially the water vapour density as a function of height. The sonde readings are not at specified heights and so the calculations of the column water and scale height to M levels (M + 1 values including the surface) must be done by quadrature as:

\[
F = \int_{z_0}^{\infty} f(z) \, dz = \sum_{j=0}^{M} w_j f(z_j)
\]

where \(f\) is some quantity being integrated and the \(w_j\) are quadrature weights. We have used the trapezoidal approximation:

\[
h_j = z_j - z_{j-1} \\
w_0 = h_1 / 2 \\
w_j = (h_{j+1} + h_j) / 2 \quad j = 1, M - 1 \\
w_M = h_M / 2.
\]

The resulting information of interest for the Wagga station is summarised in Table 3 below. There are slight differences in the water vapour at the surface from the previous section due to timing and location.

### Table 3: Summary of profile data at the Wagga station

<table>
<thead>
<tr>
<th>Radiosonde Summary</th>
<th>January 11</th>
<th>January 12</th>
<th>January 13</th>
</tr>
</thead>
<tbody>
<tr>
<td>(W [cm])</td>
<td>1.575</td>
<td>1.340</td>
<td>1.068</td>
</tr>
<tr>
<td>(H_w [km])</td>
<td>1.787</td>
<td>2.896</td>
<td>2.187</td>
</tr>
<tr>
<td>(\rho_w(z_0) [g , m^{-3}])</td>
<td>8.81</td>
<td>4.63</td>
<td>4.89</td>
</tr>
</tbody>
</table>

The high value for the scale height on January 12 indicates that there is some extra water vapour in the profile above the surface layer. The long term average data

\(^4\) However, the VPD is lowest on January 13. This tells the same story as the relative humidity and is more relevant to an evaporation study than for the purpose of this study.

\(^5\) The accuracies in the examples have not generally been applied in this section as data accuracy is not known but the precision presented has been selected based on the previous calculations.
(which will be described below) suggest that the scale height for water vapour under normal conditions would be about 2.1 km. This is not dissimilar to the January 13 result.

Figure 1 shows the vertical profile of air and dew point temperatures at Wagga on the morning of January 12 2002 as provided by ABoM:

![Figure 1: Vertical profile of air temperature and dew point temperature at Wagga on January 12 2002 close to 1000 AEST.](image)

The data show the presence of a moist layer at about 2 km with dry air above. The issues this creates are discussed later.

### 4.3.3 Wagga 10-year upper atmosphere statistics

Radiosonde data have been collected at Wagga for many years. Maher and Lee (1977) collected data from many Australian stations for the period 1957 to 1975 and presented the data as Upper Air Statistics for Australia. They are at the nominal hour of 2300 UTC, which is 0900 AEST at Wagga and the Wagga data were collected between the years 1965 and 1975. The data are available in the reference (Maher and Lee, 1977). The data at standard pressure levels for January at Wagga are presented in the Table 4:
Table 4: Long term January average data for Wagga (Maher and Lee, 1977)

<table>
<thead>
<tr>
<th>Height $z$ [km]</th>
<th>Pressure $P$ [mb]</th>
<th>Temperature $T_a$ [°C]</th>
<th>Mixing Ratio $M_r$ [g kg$^{-1}$]</th>
<th>Wind $U$ [m s$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.213</td>
<td>988</td>
<td>23.2</td>
<td>8.5</td>
<td>1</td>
</tr>
<tr>
<td>1.02</td>
<td>900</td>
<td>16.9</td>
<td>6.8</td>
<td>3</td>
</tr>
<tr>
<td>1.51</td>
<td>850</td>
<td>14.6</td>
<td>6.0</td>
<td>3</td>
</tr>
<tr>
<td>3.12</td>
<td>700</td>
<td>5.2</td>
<td>2.7</td>
<td>4</td>
</tr>
<tr>
<td>4.36</td>
<td>600</td>
<td>-2.1</td>
<td>1.3</td>
<td>5</td>
</tr>
<tr>
<td>5.79</td>
<td>500</td>
<td>-10.9</td>
<td>0.6</td>
<td>7</td>
</tr>
<tr>
<td>7.47</td>
<td>400</td>
<td>-22.5</td>
<td>0.1</td>
<td>9</td>
</tr>
<tr>
<td>9.52</td>
<td>300</td>
<td>-37.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>12.21</td>
<td>200</td>
<td>-54.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14.04</td>
<td>150</td>
<td>-60.6</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16.52</td>
<td>100</td>
<td>-67.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>17.86</td>
<td>80</td>
<td>-66.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>18.68</td>
<td>70</td>
<td>-64.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>19.62</td>
<td>60</td>
<td>-62.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20.75</td>
<td>50</td>
<td>-59.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>22.17</td>
<td>40</td>
<td>-55.9</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The water vapour data were provided as median mixing ratio but only to levels where sufficient data had been collected for a stable average. The standard deviation of the mixing ratio was not provided. Using Case 1 above and computing the other formulae the following results up to 7.5 km were obtained:

Table 5: Derived water vapour information from Table 4

<table>
<thead>
<tr>
<th>$\rho_w$ [g m$^{-3}$]</th>
<th>$\rho'_w$ [g m$^{-3}$]</th>
<th>RH [%]</th>
<th>$e_a$ [kPa]</th>
<th>$e'(T_a)$ [kPa]</th>
<th>$D$ [kPa]</th>
<th>$T_d$ [°C]</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.74</td>
<td>20.80</td>
<td>46.8</td>
<td>1.332</td>
<td>2.845</td>
<td>1.513</td>
<td>11.21</td>
</tr>
<tr>
<td>7.27</td>
<td>14.38</td>
<td>50.6</td>
<td>0.973</td>
<td>1.926</td>
<td>0.953</td>
<td>6.57</td>
</tr>
<tr>
<td>6.12</td>
<td>12.51</td>
<td>48.9</td>
<td>0.812</td>
<td>1.663</td>
<td>0.850</td>
<td>3.98</td>
</tr>
<tr>
<td>2.36</td>
<td>6.88</td>
<td>34.2</td>
<td>0.303</td>
<td>0.885</td>
<td>0.582</td>
<td>-9.28</td>
</tr>
<tr>
<td>1.00</td>
<td>4.19</td>
<td>23.9</td>
<td>0.125</td>
<td>0.524</td>
<td>0.399</td>
<td>-19.96</td>
</tr>
<tr>
<td>0.40</td>
<td>2.20</td>
<td>18.1</td>
<td>0.048</td>
<td>0.266</td>
<td>0.218</td>
<td>-30.43</td>
</tr>
<tr>
<td>0.06</td>
<td>0.87</td>
<td>6.4</td>
<td>0.006</td>
<td>0.100</td>
<td>0.094</td>
<td>-49.52</td>
</tr>
</tbody>
</table>

A plot of the temperature and dew point for the levels included in the average (and those above it where it may be argued that the dew point temperature based on the humidity sensor (hygristor) of the radiosonde is not very accurate) can be created (Figure 2) which has a similar form to the daily data:
However, any inaccuracy in the humidity at high levels has little significant effect on the total column water vapour density and for January the water vapour data of special interest can be computed and summarised as follows:

Table 6: Summary data for Wagga – 10-year January average

<table>
<thead>
<tr>
<th>Radiosonde Summary</th>
<th>January</th>
</tr>
</thead>
<tbody>
<tr>
<td>$W \ [cm]$</td>
<td>2.048</td>
</tr>
<tr>
<td>$H_w \ [km]$</td>
<td>2.103</td>
</tr>
<tr>
<td>$\rho_w(z_0) \ [g \ m^{-3}]$</td>
<td>9.74</td>
</tr>
</tbody>
</table>

The long term average atmosphere for the site is therefore moister than was found in the January 11-13 2002 radiosondes and the water vapour density at the ground is also greater in the long term average. The mean value of the water vapour scale height ($H_w$) reinforces the conclusions of the previous section as well supporting the common use of scale height at 2 km as defaults for both water vapour and aerosol.

The long term data can provide a convenient base against which to discuss the results obtained on January 12. Figure 3 plots the water vapour density for the long term average and the daily data as well as the estimated profile based on the January 12 surface water vapour density and the long term scale height.
Figure 3: Water vapour density for Wagga January 12 compared with long term average and average scale height.

Figure 3 shows the January 12 profile of water vapour density to 10 km (red line with squares marked rho_w) as well as the long term average (green line marked Rhow) plus the exponential model using the long term average scale height and the actual surface water vapour density (blue line with squares marked Est_Rhow2). The profile on the day is basically dry but with a significant moist layer between 1.5 and 2 km ASL. The moist layer breaks up the predictability of W from the surface. The main issue in this case is then whether the recorded profile applies to Coleambally or not?

Figure 4: 10-year average column water, scale height and upper bound on column water over the year for Wagga.

Before considering this question, it is interesting to use the long term data to look at the variations in mean column water vapour and scale height over the year. Figure 4
also plots the integral of the saturated water vapour ($W^*$) to provide a strict upper limit on the precipitable water ($W$) and also the scale height for water vapour ($H_w$) over the year.

It seems from Figure 4 that the scale height ($H_w$) is stable at about 2 km except for a slight reduction between August and October. The water vapour and the upper bound both follow the seasonal trend in air temperature.

### 4.4 Meteorological data at Coleambally

#### 4.4.1 Weather station data at Coleambally

For a period of the afternoon from 1600 AEST on the previous day of January 11 and over the day of January 12 until 1600 AEST, a weather station constructed by CSIRO EOC logged the surface meteorology at Coleambally. The data collected by the system are wind speed ($U$) [Km h$^{-1}$], relative humidity ($RH$) [%], solar radiation ($S$) [Wm$^{-2}$], PAR diffuse [$\mu$mol m$^{-2}$], and PAR total [$\mu$mol m$^{-2}$]. Data are reduced by the system and stored in spreadsheet compatible form.

The surface pressure is not measured by this system so the Wagga value of 98 kPa was used. By means of comparison, the long term average surface pressure for Wagga in January provided by Maher and Lee (1977) is 98.8 kPa and the formula provided in the text as a default method to compute a pressure at given elevation provides a value of 98.79 kPa. So, local knowledge is useful but not critical in this case.

![Figure 5: Solar radiation (W m$^{-2}$) measured at Coleambally on January 11-12 2002 by EOC weather station compared with published clear sky model.](image)

To reinforce the general statements of the previous section regarding the weather conditions near to the mission, Figure 5 plots the shortwave solar radiation in [W m$^{-2}$]
for the period as measured by the EOC weather station. The model labelled “S” is similar to the average clear day model for solar radiation observed at Aspendale given by Paltridge and Platt (1976).

The rapid reductions in transmittance on the afternoon of January 11 are likely due to the smoke that was reported at Wagga but January 12, after the change overnight, is a clear day with high transmittance. There is a slight problem that may be due to the instrument not being quite level but the agreement is basically very good.

![Figure 6a: Air temperature and dew point for Coleambally on January 11/12](image6a.png)

Since the given information relevant to the water vapour is air temperature, humidity and pressure the vapour calculations are the Case 2. Some results from the output series can be seen in Figures 6a and 6b which plot the air temperature and dew point temperature and a plot of the calculated vapour density as a function of time.

![Figure 6b: Surface water vapour density](image6b.png)

At the time of the overpass of the various satellites (close to 1000 AEST) relevant water vapour data were:

<table>
<thead>
<tr>
<th>Table 7: Surface data at 1000 AEST at Coleambally on January 12</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Air Temperature [°C]</strong></td>
</tr>
<tr>
<td><strong>Dew Point Temperature [°C]</strong></td>
</tr>
<tr>
<td><strong>Water Vapour Density [g m⁻³]</strong></td>
</tr>
</tbody>
</table>

That is, the air temperature measurement is a bit lower than Wagga, the dew point temperature is higher and the water vapour density is higher. This implies that there is more near surface water vapour at Coleambally than Wagga at that time but the conditions are similar based on these data and the big overnight change is also as clear in the Coleambally data record as it was in the Wagga surface data. The rapid changes late on January 11 at Coleambally, when winds moved from the west to the south, are also associated with big changes in visibility and changing air masses but their exact causes are not entirely clear.

It is possible to convert the water vapour density to apparent column water if the scale height is known. By assuming the scale height is the long term average (2.103 km) we
can estimate the column water over any of the periods of interest. Some validation for the estimate is available from the CIMEL sun photometer data that were also available at the time and the surface based estimates will be compared with the data below.

![Figure 7a: Aerosol Optical Thickness (AOT) at 550 nm](image1)

![Figure 7b: Atmospheric column precipitable water vapour (cm)](image2)

### 4.4.2 CIMEL data

The CIMEL data are available through the AERONET (AErosol RObotic Network) system (Holben et al., 1998, 2001; or see [http://aeronet.gsfc.nasa.gov/](http://aeronet.gsfc.nasa.gov/)) and provide estimates of aerosol optical depth in various spectral bands plus an estimate of the column water vapour estimated from absorption in the band centred at 936 nm. Figures 7a and 7b show the aerosol optical thickness (AOT) at 550 nm and the estimated column water vapour (cm of precipitable water) for the days in question (the x-axis is in fractional local time year days):

If the ranges of the data are focused to the day of the overpasses (January 12 2002), as shown in Figures 8a and 8b, the variation suggests a clear day with dry air – in agreement with the other data.

![Figure 8a: AOT at 550 nm for January 12.](image3)

![Figure 8b: W (cm) for January 12](image4)

The CIMEL data shows a good level of agreement with the data obtained from the weather station and the Wagga radiosondes. The rapid and dramatic changes in AOT
on January 11 (Figure 7a) follow the movement of the smoke in and away from the site. The morning of the overpasses was exceptionally clear (visibilities possibly 60 to 100 km) and the air very dry until the afternoon (Figure 8b).

Over the same periods as the Wagga radiosondes were flown, the CIMEL provides the following summary statistics that agree well with the overall regional data:

<table>
<thead>
<tr>
<th>CIMEL Summary</th>
<th>January 11</th>
<th>January 12</th>
<th>January 13</th>
</tr>
</thead>
<tbody>
<tr>
<td>$W$ [cm] (SD)</td>
<td>1.624</td>
<td>1.09 (0.05)</td>
<td>1.364</td>
</tr>
<tr>
<td>AOT550 (SD)</td>
<td>0.117</td>
<td>0.039 (0.005)</td>
<td>0.038</td>
</tr>
</tbody>
</table>

The CIMEL data provide a useful means of tracking the column water vapour. The data seem to agree well with analyses of the images taken on the day as well. Using the “FLAASH” software to atmospherically correct Hyperion data imaged on January 12, 2002, the water vapour estimates based on the satellite data at about 1000 AEST were 0.995 g cm$^{-2}$ with a SD of 0.068 g cm$^{-2}$. This is similar to the CIMEL value and the temporal variance in the CIMEL data (0.03 g cm$^{-2}$) is similar to the observed spatial variance in the Hyperion image.

The question of how well the surface data estimate the column water vapour can be considered by comparing the CIMEL column estimates with the scaled surface data. As described above, the scale height ($H_w$) we have used in this case is the long term January average for Wagga of 2.103 km. Alternatively, the ratio of the CIMEL column water vapour to the surface water vapour density can be looked at as an estimate for the scale height. These are plotted in Figure 9.

![Figure 9: CIMEL (WV_C) and surface based (W_ws) estimates for column water vapour plus estimated scale height (H_w(C))](image)
The estimate based on the weather station data (label W_ws) is close to the CIMEL estimates (label WV_C) around the time of the overpasses (1000 AEST) but diverges as the afternoon progresses. The estimated scale height (label H_w(C)) shows a progressive change from values near 2 km to values near 3 km by the late afternoon. This afternoon value is similar to the scale height at Wagga during the morning. It suggests that a moist layer that was not present in the morning moved into the Coleambally area during the day. However, with the wind pattern at the time it is unlikely to have been the same air mass that was present at Wagga during the morning. The water vapour “aloft”, despite the existence of useful correlations, is clearly not always predictable from surface measurements.

4.5 Summary of outcomes of the estimates and computations

The frontal passage on the afternoon of January 11 resulted in very clear and dry air being over the Coleambally site. The winds were quite high (the mean wind speed from the EOC weather station between 0930 and 1030 on January 12 was 26.4 km h⁻¹ from the south and steady) and, while there were changes occurring over the period during which fieldwork progressed, overall the air was clear and dry and ideal for the validation mission.

On the morning of January 12, the Wagga radiosonde showed a relatively dense layer of moist air to be present at about 2 km. This is shown by the increase in water vapour scale height at the station. However, it seems that this moist layer was not present at Coleambally on the morning of January 12. At Coleambally, the long-term average scale height and the local value seem quite close during the morning. However, over the day of January 12, it is likely that a (possibly different) moist layer arrived at Coleambally during the afternoon as is suggested by the comparison between the surface water vapour density and the CIMEL based column water vapour estimates.

It therefore seems from this simple study that none of the methods alone provided a complete solution to the needs of calibration and validation on this occasion. The Wagga radiosonde at the time of the overpass was not appropriate to Coleambally as a means of providing the water vapour profile, the surface data could be scaled effectively at the time of the overpass but from the later behaviour the success seems fairly risky for a general strategy and the CIMEL by itself does not provide profile information. The combination of the CIMEL and the local surface data seems to provide the best option since both column water and scale height are obtained.

This example is certainly not claimed to be a definitive study of estimating water vapour amount and profile to support remote sensing studies. It has only served to show the value and need of being able to transform between the different measures of water vapour (such as recorded humidity, mixing ratio or dew point temperature and output water vapour density). Some of the measures provided in the text (such as vapour pressure and vapour pressure deficit) have not been used (expect in intermediate calculations) and their use would certainly be more visible if calculations of reference evaporation had been made (as they can) using the weather station data. People who wish to carry out these calculations will quickly recognise the appropriate forms of water vapour data among the selections. In the last year the wet-bulb
formulae have also been of particular use at another site to convert observed surface data at a local site to similar data.

5 Acknowledgements

The collection of the formulae in this report started when in the late 1980s I needed to convert mixing ratio to vapour density and other quantities and Jetse Kalma (then at CSIRO Division of Water Resources) offered to find the best formulae. He came back after a longer time than he expected with the statement that there seemed to be nowhere to find the appropriate formulae all in one place and in the form needed to put into a spreadsheet. Since then the collected formulae have grown in scope and things have also changed with regard to accessibility (as evidenced by the web sites listed in the Appendix) but not to the point where the collection presented here is no longer needed by me and (I hope) by others who will use it. As well as Jetse, many people have added their knowledge whom I unfortunately cannot list in full. But Tim McVicar, Tom Van Niel (CSIRO Land and Water) and Bisun Datt (CSIRO EOC) are to be thanked for their hard work that brought together the example from the Coleambally remote sensing mission and Denis O’Brien (CSIRO Atmospheric Research) is to be thanked for his efforts in reading the document as an internal reviewer and adding significantly to its accuracy and utility. Elsevier Ltd also kindly gave permission to reproduce the excellent Table A1.2 of the Appendix 1 from Principles of Environmental Physics by J.L. Monteith and M.H. Unsworth.
6 References


7 Appendix 1: Discussion of units and less common measures of water vapour

7.1 Basics

Except for relative quantities such as percent humidity, all of the values that we derive depend on the units of the measurement. Pressure in millibars \([\text{mb}]\) or hecto-pascals \([\text{hPa}]\), temperature in degrees Celsius \([\degree \text{C}]\) or in Kelvin \([\text{K}]\), density in grams per cubic metre \([\text{g m}^{-3}]\) or kilograms per cubic metre \([\text{kg m}^{-3}]\) can be found among the data that will present themselves or in papers or books about the subject.

Scientific units are based on the basic dimensions of length, mass and time in primary metric units of metre, gram and second. However, the accepted systems of units generally use powers of 10 of the primary units of length, mass and time as in the centimetre, gram, second (cgs) system or the Metre, Kilogram, Second (MKS) system. Among the various systems in use, the SI (Système International) system has become the nearest to a universal scientific standard. It is the MKS system together with units of electric current (ampere, [\text{A}]), temperature (Kelvin, [\text{K}]), amount of substance (mole, [\text{mol}]) and luminous intensity (candela, [\text{cd}]). In addition it makes a range of choices of derived units as standards for pressure, energy, power and other quantities. It is described clearly in the Appendix A.1 of Monteith and Unsworth (1990).

Since anyone using this text will come across many forms of units we have provided two tables to help with unit conversions and definitions. The first is the basic nomenclature for the powers of 10 that are used to scale the basic units of any (metric) system. They are provided in Table A1.1 which also provides an example of the conversion:

<table>
<thead>
<tr>
<th>Name</th>
<th>Symbol</th>
<th>Power</th>
<th>One Unit =</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tera</td>
<td>T unit</td>
<td>10^{12}</td>
<td>10^{-12} tera-unit</td>
</tr>
<tr>
<td>Giga</td>
<td>G unit</td>
<td>10^9</td>
<td>10^{-9} giga-unit</td>
</tr>
<tr>
<td>Mega</td>
<td>M unit</td>
<td>10^6</td>
<td>10^{-6} mega-unit</td>
</tr>
<tr>
<td>Kilo</td>
<td>k unit</td>
<td>10^3</td>
<td>10^{-3} kilo-unit</td>
</tr>
<tr>
<td>Hecto</td>
<td>h unit</td>
<td>10^2</td>
<td>10^{-2} hecto-unit</td>
</tr>
<tr>
<td>Deca</td>
<td>da unit</td>
<td>10^1</td>
<td>10^{-1} deca-unit</td>
</tr>
<tr>
<td>[Unit]</td>
<td>[unit]</td>
<td>10^0</td>
<td>1 unit</td>
</tr>
<tr>
<td>Deci</td>
<td>d unit</td>
<td>10^{-1}</td>
<td>10 deci-unit</td>
</tr>
<tr>
<td>Centi</td>
<td>c unit</td>
<td>10^{-2}</td>
<td>10^{-2} centi-unit</td>
</tr>
<tr>
<td>Milli</td>
<td>m unit</td>
<td>10^{-3}</td>
<td>10^{-3} milli-unit</td>
</tr>
<tr>
<td>Micro</td>
<td>\mu unit</td>
<td>10^{-6}</td>
<td>10^{-6} micro-unit</td>
</tr>
<tr>
<td>Nano</td>
<td>n unit</td>
<td>10^{-9}</td>
<td>10^{-9} nano-unit</td>
</tr>
<tr>
<td>Pico</td>
<td>p unit</td>
<td>10^{-12}</td>
<td>10^{-12} pico-unit</td>
</tr>
</tbody>
</table>

While it is easy enough to cope with the fact that since 1 cm is 1/100th of a metre you need to multiply values in metres by 100 to get the result in cm it is not so obvious to establish with certainty whether to convert data in \(\mu W \text{ cm}^{-2} \text{ nm}^{-1} \text{ sr}^{-1}\) to...
\( W \text{ } m^{-2} \mu m^{-1} sr^{-1} \) (the SI units for radiance) you need to multiply by 10 or divide by 10. The above Table A1.1 and the following one, Table A1.2 – which is taken from Appendix A1 of Monteith and Unsworth (1990) – can help you to decide.

The Table A1.2 from Monteith and Unsworth (1990) has the units reduced to dimensions of length, mass and time as well as direct and understandable comparisons between SI and cgs system units. If the tables included here are not sufficient to answer your questions then a good source of information on this and units generally can be found at:

http://www.ex.ac.uk/cimt/dictunit/dictunit.htm

7.2 Units for water vapour

The units used in this document for water vapour measures are generally a mix of cgs and SI units. The choices conform mostly with the choices made by Smith et al. (1992). The units are commonly used and well known in the field of micrometeorology. The choice of units is difficult since the use of SI units has the advantage of universal standardisation but is not yet universally used. Temperature in °C and K are equally acceptable in the practice of SI units although K is officially the SI choice. However, the situation in other cases is that units are generally chosen in a way that provides numbers of convenient size and range for the conditions of their use. Furthermore, in activities involving water vapour, convenience in size and range often stems from the underlying fact that one cc (cubic cm or \( cm^3 \)) of liquid water has mass of (very close to) one gram [g]. This fact (still) gives the cgs system a role in water vapour units.

There are some occasions in the text when we have avoided the conventional but still do not use SI. This is the case in pressure where the very common millibars \( [mb] \) gives the same number as hectoPascals \( [hPa] \) but we have chosen to use kiloPascals \( [kPa] \) since it is commonly used in micrometeorology. That is, 1013.25 \( mb \) is “one atmosphere” or 1013.25 \( hPa \) or 101.325 \( kPa \). Since it is important at least to relate the units used in the text to SI units we have therefore provided a Table A1.3 of the relationships:

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Units in text</th>
<th>Example</th>
<th>SI Units</th>
<th>Equivalent SI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure ( P )</td>
<td>k Pa</td>
<td>101.325</td>
<td>Pa</td>
<td>1.01325 x 10^5</td>
</tr>
<tr>
<td>Density ( \rho_w )</td>
<td>g ( m^{-3} )</td>
<td>4.27</td>
<td>kg ( m^{-3} )</td>
<td>4.27 x 10^{-3}</td>
</tr>
<tr>
<td>Mixing ratio ( m_r )</td>
<td>g ( kg^{-1} )</td>
<td>7.64</td>
<td>kg ( kg^{-1} )</td>
<td>7.64 x 10^{-3}</td>
</tr>
<tr>
<td>Vapour pressure ( e_a )</td>
<td>k Pa</td>
<td>1.206</td>
<td>Pa</td>
<td>1.206 x 10^3</td>
</tr>
</tbody>
</table>

It is not difficult, based on this table, to modify the formulae or the results if the SI units are desired. However, it is the size and range of the units that has led to the choice of the mixed units.
Table A1.2 Système International (SI) units with c.g.s. equivalents (from Principles of Environmental Physics by J.L. Monteith and M.H. Unsworth, 1990. Reprinted by permission of Elsevier Ltd)

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Dimensions</th>
<th>SI</th>
<th>c.g.s.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length</td>
<td>L</td>
<td>1 m</td>
<td>$= 10^{2}$ cm</td>
</tr>
<tr>
<td>Area</td>
<td>L²</td>
<td>1 m²</td>
<td>$= 10^{4}$ cm²</td>
</tr>
<tr>
<td>Volume</td>
<td>L³</td>
<td>1 m³</td>
<td>$= 10^{6}$ cm³</td>
</tr>
<tr>
<td>Mass</td>
<td>M</td>
<td>1 kg</td>
<td>$= 10^{3}$ g</td>
</tr>
<tr>
<td>Density</td>
<td>M L⁻³</td>
<td>1 kg m⁻³</td>
<td>$= 10^{-3}$ g cm⁻³</td>
</tr>
<tr>
<td>Time</td>
<td>T</td>
<td>1 s (or min, h, etc.)</td>
<td>$= 1$ s</td>
</tr>
<tr>
<td>Velocity</td>
<td>L T⁻¹</td>
<td>1 m s⁻¹</td>
<td>$= 10^{2}$ cm s⁻¹</td>
</tr>
<tr>
<td>Acceleration</td>
<td>L T⁻²</td>
<td>1 m s⁻²</td>
<td>$= 10^{2}$ cm s⁻²</td>
</tr>
<tr>
<td>Force</td>
<td>M L T⁻²</td>
<td>1 kg m s⁻² = 1 N (Newton)</td>
<td>$= 10^{5}$ g cm s⁻² $= 10^{5}$ dynes</td>
</tr>
<tr>
<td>Pressure</td>
<td>M L⁻¹ T⁻²</td>
<td>1 kg m⁻¹ s⁻² = 1 N m⁻² (Pascal)</td>
<td>$= 10$ g cm⁻¹ s⁻² $= 10^{2}$ mbar</td>
</tr>
<tr>
<td>Work, energy</td>
<td>M L² T⁻²</td>
<td>1 kg m² s⁻² = 1 J (Joule)</td>
<td>$= 10^{7}$ g cm² s⁻² $= 10^{7}$ ergs</td>
</tr>
<tr>
<td>Power</td>
<td>M L² T⁻³</td>
<td>1 kg m² s⁻³ = 1 W (Watt)</td>
<td>$= 10^{7}$ g cm² s⁻³ $= 10^{7}$ ergs s⁻¹</td>
</tr>
<tr>
<td>Dynamic viscosity</td>
<td>M L⁻¹ T⁻¹</td>
<td>1 N s m⁻²</td>
<td>$= 10$ dynes s cm⁻² $= 10$ Poise</td>
</tr>
<tr>
<td>Kinematic viscosity</td>
<td>L² T⁻¹</td>
<td>1 m² s⁻¹</td>
<td>$= 10^{4}$ cm² s⁻¹ $= 10^{4}$ Stokes</td>
</tr>
<tr>
<td>Temperature</td>
<td>H (or M L² T⁻²)</td>
<td>1 °C (or 1 K)</td>
<td>$= 1$ °C (or 1 K)</td>
</tr>
<tr>
<td>Heat energy</td>
<td>H T⁻¹</td>
<td>1 J</td>
<td>$= 0.2388$ cal</td>
</tr>
<tr>
<td>Heat or radiation flux</td>
<td>H L⁻² T⁻¹</td>
<td>1 W</td>
<td>$= 0.2388$ cal s⁻¹</td>
</tr>
<tr>
<td>Heat flux density</td>
<td>H M⁻¹</td>
<td>1 W m⁻²</td>
<td>$= 2.388 \times 10^{-5}$ cal cm⁻² s⁻¹</td>
</tr>
<tr>
<td>Latent heat</td>
<td>H M⁻¹ θ⁻¹</td>
<td>1 J kg⁻¹</td>
<td>$= 2.388 \times 10^{-4}$ cal g⁻¹</td>
</tr>
<tr>
<td>Specific heat</td>
<td>H M⁻¹ θ⁻¹</td>
<td>1 J kg⁻¹ K⁻¹</td>
<td>$= 2.388 \times 10^{-4}$ cal g⁻¹ K⁻¹</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>H L⁻¹ θ⁻¹ T⁻¹</td>
<td>1 W m⁻¹ K⁻¹</td>
<td>$= 2.388 \times 10^{-3}$ cal cm⁻¹ s⁻¹ K⁻¹</td>
</tr>
<tr>
<td>Thermal diffusivity (and other diffusion coefficients)</td>
<td>L² T⁻¹</td>
<td>1 m² s⁻¹</td>
<td>$= 10^{-4}$ cm² s⁻¹</td>
</tr>
</tbody>
</table>
7.3 Less common units

There are some other units that will be encountered by people using water vapour data and (in some cases) desired by them as being appropriate to a particular problem. Not everyone may agree that the following measures are “uncommon” but to people who work in Earth Observation they generally are – unless they are dealing with radiative transfer code at the fundamental level. Whatever the case, they are easily derived from measures already computed and the conversion factors are listed in this section.

For example, the MODTRAN computer code (Berk et al., 1999) accepts user input of atmospheric profiles and for the water vapour profile accepts data in the following units:

- Volume mixing ratio [ppmv]
- Number density [molecules cm\(^{-3}\)]
- Mass mixing ratio \((m_r)\) [g kg\(^{-1}\)]
- Vapour density \((\rho_w)\) [g m\(^{-3}\)]
- Vapour pressure \((e_a)\) [mb or hPa]
- Dew point temperature \((T_d)\) [°C or K]
- Relative humidity \((RH)\) [%]

Users of the FLAASH software (which is based on Modtran 4) for atmospheric correction will also find that the column water vapour results are output in “atmosphere centimetres” [atm cm] as are outputs in Modtran. It is used by the FLAASH software as the units for the output image estimating column water vapour for each pixel.

Five of the units listed above for the possible Modtran inputs, including and after the mass mixing ratio, are the same as in this text except that vapour pressure is in hPa rather than kPa. The others are the Volume mixing ratio (VMR), which can also be called mole ratio, and number density (ND). These can certainly be used to express water vapour amount but are perhaps more commonly used for non-condensable gases such as CO\(_2\). The expressions can be related to the ones used in the text using the ideal gas equation (Eqs 1,2).

7.3.1 Volume mixing ratio (mole fraction)

The volume mixing ratio is the ratio of the number of moles of water vapour to the number of moles of dry air. Expressed as parts of water vapour by volume per million parts of dry air (ppm) we have:

\[
PPM_v = 10^6 \frac{e_a}{P - e_a} = \frac{10^6}{0.62198} m_r
\]
Water Vapour Measures

where \( m_r \) is the mass mixing ratio described in the text and the factor 0.62198 is the ratio of the relative molar masses of water and dry air \( (M_w / M_A) \).

### 7.3.2 Number density

For the number density in molecules \( cm^{-3} \) we find that:

\[
ND = N_A \frac{e_a}{R(T_a + T_0)} = N_A \frac{\rho_a}{M_w}
\]

where besides expressions that have been previously defined, the constant \( N_A \) is the number of molecules in one mole of gas or the Avagadros Number \( (6.0221367 \times 10^{23}) \). That is, these forms of water vapour amount are easily inter-converted with those used in the text.

### 7.3.3 Atmosphere centimetres

One atmosphere centimetre \( (atm-cm) \) at STP is equivalent to a length of 1 \( cm \) of gas at STP (temperature in Kelvin at the ice point (zero \( ^\circ C \) or 273.15 \( K \)) and pressure at one atmosphere or 101.325 \( kPa \)) per \( cm^2 \). This is a definition that suits any gas and in its computation gases are reduced to equivalent STP along the path. To relate the column water vapour in \( atm-cm \) to \( cm \) of precipitable water or (equivalently) column water in \( g \ cm^{-2} \) we need to make use of the molar volume \( (V_m) \) at STP. At STP the molar volume of any gas is:

\[
V_{m0} = \frac{RT_0}{P_0} = 22.41359 \text{ Litres} = 2.241359 \times 10^4 \text{ cm}^3.
\]

Using the definition of \( atm-cm \) above for water vapour:

\[
1 \ atm-cm = \frac{M_w}{V_{m0}} \ g \ cm^{-2} = 8.037686E-04 \ g \ cm^{-2} \\
1 \ g \ cm^{-2} = 1244.139 \ atm-cm.
\]

That is, the units for column water vapour can also be easily converted to one another by using these factors. The factors also provide another example of how units are chosen to be convenient in size and range. Column water vapour in \( atm-cm \) is used directly as an output (integer) image in FLAASH. Multiplying \( cm \) of precipitable...
water (i.e. \( g \ cm^{-2} \) of water vapour) by 1000 would not be quite the same precision. However, the difference would not be very serious.

### 7.3.4 Specific humidity \((q)\)

The final unit that is worth mentioning in this Appendix is the specific humidity \((q)\). As noted in the previous discussion, density of water vapour \((\rho_w)\) is the ratio of mass of water vapour per unit volume of moist air and is sometimes called the “absolute humidity”. “Specific humidity” (see Garratt, 1992, Appendix 2) is the mass of water vapour per unit mass of moist air and is closely related to the mass mixing ratio.

The density of moist air \((\rho_a)\) is the sum of densities of water vapour \((\rho_w)\) and dry air \((\rho_d)\) and from the expressions developed previously in the discussions of water vapour density and mass mixing ratio it follows that:

\[
q = \frac{\rho_w}{\rho_a} = \frac{\varepsilon e_a}{(P - e_a) + \varepsilon e_a} = \frac{\varepsilon e_a}{P - (1 - \varepsilon)e_a} = \frac{m_e}{1000 + m_e}
\]

where the mixing ratio is in \(g \ kg^{-1}\). The constant \(\varepsilon\) is (as previously) the ratio of the molar masses of water and dry air. This unit is, in view of its relationships with water vapour density and mixing ratio not normally needed and can be claimed to be “uncommon”. However, it is sometimes used in the definition of precipitable water in the form:

\[
W = \frac{1}{g} \int_0^h q \, dP
\]

where \(g\) is acceleration due to gravity (approximately 9.8 \(m \ s^{-2}\)). This is identical with the preceding expression under hydrostatic equilibrium where:

\[
\frac{dP}{dz} = -\varepsilon \rho_a(z).
\]

If there are still other units and expressions that you come across and wish to find even more information it should be able to be found at the web site listed above or at one of many others, such as:

http://www.rotronic-usa.com/datasheets/Ref/reference.htm#Top

or

http://www.me.umn.edu/courses/me5115/notes/Introduction.pdf
Appendix 2. Computing wet-bulb temperature

In the main text, the primary concern was to derive the various water vapour parameters when the wet-bulb temperature ($T_w$) is an input together with the dry-bulb ($T_d$).

The psychrometric equation is:

$$e_a = e^*(T_w) - \gamma(T_d - T_w)$$

where the terms were derived and defined in the main text. Clearly, if the quantities $T_w$ and $T_d$ are known then a solution for $e_a$ is straightforward to obtain.

There are three approaches to inverting the equation (that is, to obtain $T_w$ when $e_a$ is known) that we will consider. These are linearisation, fixed point iteration and nonlinear equation solving. The first of these is easy to implement, the second is easy enough in a spreadsheet while the third really needs to be implemented in a computer program. However, the second and third both converge quickly if care is taken.

**8.1 Linearisation:**

Linearising $e^*$ about $T_d$ we obtain:

$$e^*(T_w) \approx e^*(T_d) + \frac{\partial e^*}{\partial T}
\bigg|_{T_d} (T_w - T_d)$$

$$= e^*(T_d) + \Delta(T_w - T_d)$$

Hence:

$$e^*(T_d) - e_a = D$$

$$\approx (\gamma + \Delta)(T_d - T_w)$$

or

$$T_w \approx T_d - \frac{D}{\gamma + \Delta}.$$ 

This is an easily computed estimate for the wet-bulb temperature. However, it is not very accurate for low humidity conditions (such as $RH < 30\%$). If it is important for the result to be exact then one of the following two should be used.

**8.2 Fixed point iteration**

We can write the psychrometric equation in the form:
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\[ T_w = F(T_w) \]
\[ = T_a - \frac{1}{\gamma} (e^*(T_w) - e_a) \]

This provides a fixed-point iteration of the form:

\[ T_{wj} = F(T_{w(j-1)}) \]

The above linearised approximation can obviously provide a good starting value for the iteration.

\[ T_{w0} = T_a - \frac{D}{\gamma + \Delta} \]

It is, however, found that this is unstable and/or converges slowly for low to very low humidity conditions and some temperature ranges. The convergence can be made faster (e.g. two or three iterations normally being sufficient) and the solution stable even at low humidity (e.g. RH < 30%) with the modification:

\[ T'_{wj} = F(T_{w(j-1)}) \]
\[ T_{wj} = (T_{w(j-1)} + T'_{wj}) / 2. \]

Again, this is quite straightforward to implement in a spreadsheet without invoking the “circular” reference option.

8.3 Nonlinear equation solving

The full nonlinear system corresponds to finding a zero of a nonlinear function as in:

\[ f(T_w) = e_a - e^*(T_w) + \gamma(T_a - T_w) \]
\[ = 0. \]

Note that:

\[ f'(T) = -(\gamma + \Delta) + (T_a - T) \frac{\partial \gamma}{\partial T} \]
\[ = -(\gamma + \Delta) + 2.361 \times 10^{-3} \frac{\gamma}{\lambda} (T_a - T) \]

where \( \Delta \) is evaluated at the current value of \( T \).

This can be quickly solved by a Newton search from the previous linearised solution \( (T_{w0}) \) as starting point with a final iteration not involving derivatives and will converge as quickly as the fixed-point iteration or even faster. However, as noted above, it is not well suited to a spreadsheet.
9 Appendix 3: Derivatives for standard deviations for the measures

The following sets of derivatives are used as described in the text to compute approximate standard deviations for the outputs measures of water vapour given that estimates are available or some defaults used for the standard deviations of the basic inputs, $T_a$, $P$ and one of four cases of input water vapour data denoted generally as $I_w$. In some cases, derivatives are composed of others that are assumed to be previously calculated. In many cases, only some of the three possible sources of variation are normally used in each expression.

9.1 The initial set

<table>
<thead>
<tr>
<th>Expression (no $I_w$)</th>
<th>$\frac{\partial}{\partial T_a}$</th>
<th>$\frac{\partial}{\partial P}$</th>
<th>$\frac{\partial}{\partial I_w}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e^* = 0.61078 \times e^{\frac{17.269T_a}{T_a + 237.29}}$</td>
<td>$\Delta$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$\Delta = \frac{4097.76 \times e^* (T_a)}{(T_a + 237.29)^2}$</td>
<td>$\Delta \times \left(3623.18 - 2 \times T_a \right)$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$\lambda = 2.501 - 2.361 \times 10^{-3} \times T_a$</td>
<td>$-2.361 \times 10^{-3}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$\gamma = 1.6287 \times 10^{-3} \times \frac{P}{\lambda}$</td>
<td>$2.361 \times 10^{-3} \times \frac{\gamma}{\lambda}$</td>
<td>$\frac{\gamma}{P}$</td>
<td>0</td>
</tr>
</tbody>
</table>
### 9.2 Case 1 Mixing ratio given

<table>
<thead>
<tr>
<th>Expression ($I_w = m_r$)</th>
<th>$\frac{\partial}{\partial T_a}$</th>
<th>$\frac{\partial}{\partial P}$</th>
<th>$\frac{\partial}{\partial I_w}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e_a = \frac{m_r P}{621.98 + m_r}$</td>
<td>0</td>
<td>$\frac{e_a}{P}$</td>
<td>$\frac{621.98 \times e_a}{m_r (621.98 + m_r)}$</td>
</tr>
<tr>
<td>$\rho_w = 2166.8 \frac{e_a}{(T_a + T_0)}$</td>
<td>$- \frac{\rho_w}{T_a + T_0}$</td>
<td>$\frac{\rho_w}{P}$</td>
<td>$\rho_w \frac{\partial e_a}{e_a \partial I_w}$</td>
</tr>
<tr>
<td>$RH = 100 \times \frac{e_a}{e^*(T_a) \rho}$</td>
<td>$- \frac{\Delta \times RH}{e^*(T_a)}$</td>
<td>$\frac{RH}{P}$</td>
<td>$RH \frac{\partial e_a}{e_a \partial I_w}$</td>
</tr>
<tr>
<td>$VPD = e^*(T_a) - e_a$</td>
<td>$\Delta$</td>
<td>$- \frac{e_a}{P}$</td>
<td>$- \frac{\partial e_a}{\partial I_w}$</td>
</tr>
<tr>
<td>$T_d = \frac{13.741 \times \ln(e_a) + 6.7745}{0.97145 - 0.057907 \times \ln(e_a)}$</td>
<td>0</td>
<td>$\frac{13.741 + 0.057907 \times T_d}{P \times (0.97145 - 0.057907 \times \ln(e_a))}$</td>
<td>$\frac{13.741 + 0.057907 \times T_d}{e_a \times (0.97145 - 0.057907 \times \ln(e_a)) \partial I_w}$</td>
</tr>
<tr>
<td>$T_w = T_a - \frac{VPD}{\Delta + \gamma}$</td>
<td>$\frac{\gamma + T_a - T_d}{\Delta + \gamma} \left( \frac{\partial \Delta}{\partial T_a} + \frac{\partial \gamma}{\partial T_a} \right)$</td>
<td>$\frac{1}{\Delta + \gamma} \frac{e_a}{P}$</td>
<td>$\frac{1}{\Delta + \gamma} \frac{\partial e_a}{\partial I_w}$</td>
</tr>
</tbody>
</table>
### 9.3 Case 2: Relative humidity given

<table>
<thead>
<tr>
<th>Expression ( I_w = RH )</th>
<th>( \frac{\partial}{\partial T_a} )</th>
<th>( \frac{\partial}{\partial P} )</th>
<th>( \frac{\partial}{\partial I_w} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( e_a = \frac{RH \times e^*(T_a)}{100} )</td>
<td>( RH \times \Delta )</td>
<td>0</td>
<td>( \frac{e^*(T_a)}{100} )</td>
</tr>
<tr>
<td>( \rho_w = \frac{2166.8 \times e_a}{(T_a + T_0)} )</td>
<td>( \frac{\rho_w}{e_a} \frac{\partial e_a}{\partial T_a} = \frac{\rho_w}{T_a + T_0} )</td>
<td>0</td>
<td>( \frac{\rho_w}{e_a} \frac{\partial e_a}{\partial I_w} )</td>
</tr>
<tr>
<td>( VPD = e^*(T_a) - e_a )</td>
<td>( \Delta(1 - \frac{RH}{100}) )</td>
<td>0</td>
<td>( -\frac{\partial e_a}{\partial I_w} )</td>
</tr>
<tr>
<td>( m_r = \frac{621.98 \times e_a}{P - e_a} )</td>
<td>( \frac{Pm_r}{e_a(P - e_a)} \frac{\partial e_a}{\partial T_a} )</td>
<td>( -\frac{m_r}{P - e_a} )</td>
<td>( \frac{Pm_r}{e_a(P - e_a)} \frac{\partial e_a}{\partial I_w} )</td>
</tr>
<tr>
<td>( T_d = \frac{13.741 \times \ln(e_a) + 6.7745}{0.97145 - 0.057907 \times \ln(e_a)} )</td>
<td>( \frac{13.741 + 0.057907 \times T_d \times \frac{\partial e_a}{\partial T_a}}{e_a \times (0.97145 - 0.057907 \times \ln(e_a)) \frac{\partial T_a}{\partial I_w}} )</td>
<td>0</td>
<td>( \frac{13.741 + 0.057907 \times T_d \times \frac{\partial e_a}{\partial I_w}}{e_a \times (0.97145 - 0.057907 \times \ln(e_a)) \frac{\partial T_a}{\partial I_w}} )</td>
</tr>
<tr>
<td>( T_w \approx T_a - \frac{VPD}{\Delta + \gamma} )</td>
<td>( \frac{\Delta \frac{RH}{100} + \gamma}{\Delta + \gamma} - T_a \frac{\partial \Delta}{\partial T_a} + \frac{\partial \gamma}{\partial T_a} )</td>
<td>( \frac{T_a - T_d \frac{\partial \gamma}{\partial P}}{\Delta + \gamma} )</td>
<td>( \frac{1}{\Delta + \gamma} \frac{\partial e_a}{\partial I_w} )</td>
</tr>
</tbody>
</table>
9.4 Case 3: Dew point temperature given

<table>
<thead>
<tr>
<th>Expression ($I_w = T_d$)</th>
<th>$\frac{\partial}{\partial T_a}$</th>
<th>$\frac{\partial}{\partial P}$</th>
<th>$\frac{\partial}{\partial I_w}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e_a = e^*(T_a)$</td>
<td>$0$</td>
<td>$0$</td>
<td>$\Delta</td>
</tr>
<tr>
<td>$\rho_w = 2166.8 \frac{e_a}{(T_d + T_0)}$</td>
<td>$- \frac{\rho_w}{T_d + T_0}$</td>
<td>$0$</td>
<td>$\frac{\rho_w \partial e_a}{e_a \partial I_w}$</td>
</tr>
<tr>
<td>$RH = 100 \times \frac{e_a}{e^*(T_a)}$</td>
<td>$- \frac{\Delta \times RH}{e^*(T_a)}$</td>
<td>$0$</td>
<td>$\frac{RH \partial e_a}{e_a \partial I_w}$</td>
</tr>
<tr>
<td>$VPD = e^*(T_a) - e_a$</td>
<td>$\Delta$</td>
<td>$0$</td>
<td>$- \frac{\partial e_a}{\partial I_w}$</td>
</tr>
<tr>
<td>$m_r = 621.98 \frac{e_a}{P - e_a}$</td>
<td>$0$</td>
<td>$- \frac{m_r}{P - e_a}$</td>
<td>$\frac{P m_r \partial e_a}{e_a (P - e_a) \partial I_w}$</td>
</tr>
<tr>
<td>$T_w \approx T_d - \frac{VPD}{\Delta + \gamma}$</td>
<td>$\frac{\gamma}{\Delta + \gamma} - \frac{T_d - T_a}{\Delta + \gamma} \left( \frac{\partial \Delta}{\partial T_a} + \frac{\partial \gamma}{\partial T_a} \right)$</td>
<td>$- \frac{T_d - T_a}{\Delta + \gamma} \frac{\partial \gamma}{\partial P}$</td>
<td>$\frac{1}{\Delta + \gamma} \frac{\partial e_a}{\partial I_w}$</td>
</tr>
</tbody>
</table>
## 9.5 Case 4: Wet-bulb temperature given

<table>
<thead>
<tr>
<th>Expression ($I_w = T_w$)</th>
<th>(\frac{\partial}{\partial T_a})</th>
<th>(\frac{\partial}{\partial P})</th>
<th>(\frac{\partial}{\partial I_w})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(e_a = e^*(T_w) + \gamma(T_w - T_a))</td>
<td>(-\gamma + (T_w - T_a) \frac{\partial \gamma}{\partial T_a})</td>
<td>0</td>
<td>(\Delta_{T=T_w} + \gamma)</td>
</tr>
<tr>
<td>(\rho_w = 2166.8 \frac{e_a}{(T_a + T_0)})</td>
<td>(\rho_w \frac{\partial e_a}{\partial T_a} - \frac{\rho_v}{T_a + T_0})</td>
<td>0</td>
<td>(\rho_w \frac{\partial e_a}{\partial I_w})</td>
</tr>
<tr>
<td>(RH = 100 \times \frac{e_a}{e^*(T_a)})</td>
<td>(RH \frac{\partial e_a}{\partial T_a} - RH \Delta)</td>
<td>0</td>
<td>(RH \frac{\partial e_a}{\partial I_w})</td>
</tr>
<tr>
<td>(VPD = e^*(T_a) - e_a)</td>
<td>(\Delta \frac{\partial e_a}{\partial T_a})</td>
<td>0</td>
<td>(\frac{\partial e_a}{\partial I_w})</td>
</tr>
<tr>
<td>(m_r = 621.98 \frac{e_a}{P - e_a})</td>
<td>(\frac{P_m}{e_a (P - e_a)} \frac{\partial e_a}{\partial T_a})</td>
<td>(- \frac{m_r}{P - e_a})</td>
<td>(\frac{P_m}{e_a (P - e_a)} \frac{\partial e_a}{\partial I_w})</td>
</tr>
<tr>
<td>(T_d = \frac{13.741 \times \ln(e_a) + 6.7745}{0.97145 - 0.057907 \times \ln(e_a)})</td>
<td>(13.741 + 0.057907 \times T_d) (\frac{\partial e_a}{\partial e_a})</td>
<td>0</td>
<td>(13.741 + 0.057907 \times T_d) (\frac{\partial e_a}{\partial e_a})</td>
</tr>
</tbody>
</table>
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