

Suggested Changes to the Algorithms for the Calculation of Vapor Pressure

February 21, 2011

Code Now In Use:

The equilibrium vapor pressure with respect to a water surface or an ice surface is used for some of the derived-variable calculations. At present the Goff-Gratch formulation is used, in the following form:

For measurements from dew-point hygrometers where the reading is below 0°C, the measurement is assumed to be the frost point and is converted to dewpoint using the following formula:

```
if (dp < 0.0) {dp = 0.009109+dp*(1.134055+dp*0.001038);}
```

The conversion to vapor pressure from dewpoint is then implemented in the function esubt (where “Kelvin” is 273.15):

```
static const double    Ts = 373.16, To = Kelvin;
/* ----- */
double esubt(double temperature, double pressure)
{
    double Tk = temperature + To;
    double fw, ew;
    if (Tk < 1.0) {Tk = 1.0;}
    ew = pow(10.0,
        (-7.90298 * ((Ts / Tk) - 1.0)
        +5.02808 * log10(Ts / Tk)
        -1.3816e-7 * (pow(10.0, 11.334 * (1.0 - Tk / Ts)) - 1.0)
        +8.1328e-3 * (pow(10.0, -3.49149 * (Ts / Tk - 1.0)) - 1.0))
        +log10(1013.246) );
    /* Arden Buck's pressure enhancement factor. */
    fw = 1.0007 + (3.46e-6 * pressure);
    return(ew * fw);
}
```

The procedure is thus to convert all measurements to equivalent-dew-point measurements and then to perform all subsequent calculations with the dew-point values. There are some small errors in this code and one possible improvement to be made:

1. The coefficient 11.334 should be 11.344
2. The conversion to standard atmosphere changed since the publication of the Goff-Gratch (1946) formulation, and the reference pressure should be 1013.25 instead of 1013.246. Furthermore, revised formulas were published by Goff in 1957 and 1965, although the change is not significant; see either Murphy and Koop or the web document of Voemel (<http://cires.colorado.edu/~voemel/vp.html>).
3. The correction for atmospheric pressure that enters through fw would be better represented (according to Murphy and Koop, 2005) by:

$$f = 1 + 10^{-5}p(4.923 - 0.0325T + 5.84 \times 10^{-5}T^2) \quad (1)$$

where T is the temperature in kelvin. At a pressure of 1000 mb, the Buck enhancement factor f_w is 1.00415 while (for $T=273.15$) f is 1.00403, so the difference is insignificant at that point. However, the dependence on pressure is significantly different, and no temperature dependence is included in the Buck formula. Because the formula from Buck was based on the Hyland (1975) formula that Murphy and Koop also used to obtain a better fit, it seems appropriate to change to their new formula for f . A more significant error is that the procedure being used first converts all frost-point measurements to dew-point and then uses the water enhancement factor f_w applicable for water, while even Appendix C of RAF Bulletin 9 indicates that a different correction should be used for ice. Consider the effect at $T=273.15-80=193.15$ K: The above formula gives an enhancement factor of about $1+.008(p/(1000 \text{ mb}))$ while the Buck formula gives $1+0.003(p/(1000 \text{ mb}))$. While this is a small difference in terms of values obtained for the vapor pressure, applying the wrong formula (even inconsistent with Appendix C) is an error that should be corrected. Murphy and Koop (2005) suggest using the above formula for any temperature from 180 to 330 K, where it applies to vapor pressure calculated from the frost point below $T=273.15$ but vapor pressure calculated from the dew point above $T=273.15$.

The net effect of the above changes is insignificant for dewpoints above -50°C , and is a maximum of about 0.1% at -80°C . However, there are some more important reasons for considering a change to the formulas used for vapor pressure, as discussed in the next sections.

Reasons For Recommending Revision:

- New measurements of the equilibrium vapor pressure over water and ice were made after the Goff-Gratch representation was developed, and there were various small revisions to the temperature scales and reference values on which that representation was based. For example, the publications by Wexler (1976)¹ and Wexler (1977)² presented fits that differ significantly from the Goff-Gratch formula, giving e.g. the equilibrium vapor pressure over water at 0°C ($e_{s,w}(0^\circ\text{C})$) of 6.112 mb vs 6.103 mb obtained from the Goff-Gratch formula. Flatau et al.(1992)³ emphasized the need for revision of the standard convention in use in meteorology and developed alternative fits to the modern data. See also Wagner et al., 1994.⁴
- Murphy and Koop (2005)⁵ developed a new fit to experimental data, with the significant addition that they used modern information on the specific heat and latent heat of supercooled

¹Wexler, A., 1976: Vapor pressure formulation for water in range 0 to 100°C . A revision. J. Res. Natl. Bur. Stand. Sect. A., 80, 775

²A Wexler, A., 1977: Vapor pressure formulation for ice. J. Res. Natl. Bur. Stand. A., 81, 5–20

³J. Appl. Meteorol., 31, 1507–1513

⁴Wagner, W., A. Saul and A. Pruss, 1994: International equations for the pressure along the melting and along the sublimation curve of ordinary water substance. J. Phys. Chem. Ref. Data, 23, 515-527.

⁵Q. J. R. Meteorol. Soc. (2005), 131, pp. 1539–1565

water to extend the fits for water into the supercooled region. Earlier formulas, including that of Goff and Gratch, specifically warned against extrapolation to supercooled water because of the lack of data. This work presents a justified extrapolation and a single formula valid both above and below the freezing point, as well as offering a new and simplified fit to the data for equilibrium vapor pressure over ice. Their fit in the supercooled region is significantly different from Goff and Gratch, especially for temperature around -70°C , where their equation gives an equilibrium vapor pressure of 0.479 mb vs 0.491 mb from Goff and Gratch (1946) and 0.492 mb from Goff (1965). The Murphy and Koop paper is summarized in the next section.

Murphy and Koop (2005):

Murphy and Koop (2005) presents an analysis based on integration of the Clausius-Clapeyron equation with modern data for the specific heat of supercooled water, from which one can obtain the latent heat of vaporization needed for the integration, and they extend the analysis into the supercooled-water region. They note that previous extrapolations for supercooled water were not intended for such use or justified. On the basis of fits to existing data, they present new equations for the equilibrium vapor pressure over a plane water surface and over a plane ice surface.

Frost Point

For equilibrium relative to ice, their new and relatively simple formula, plotted in Fig. 1, agrees with Goff-Gratch to within 0.2% for temperatures from -100 to 0°C , with theirs 0.2% higher at the low limit. The formula is equivalent to the following equation for the equilibrium vapor pressure with respect to a plane ice surface ($e'_{s,i}$) in terms of the absolute temperature T of the frost point:⁶

$$e_{s,i} = b'_0 \exp\left(b_1 \frac{(T_0 - T)}{T_0 T} + b_2 \ln\left(\frac{T}{T_0}\right) + b_3 (T - T_0)\right) \quad (2)$$

where $T_0 = 273.15 \text{ K}$, $b_0 = 9.550426$, $b_1 = -5723.265 \text{ K}$, $b_2 = 3.53068$, $b_3 = -0.00728332 \text{ K}^{-1}$, and $b'_0 = \left(\frac{1 \text{ hPa}}{100 \text{ Pa}}\right) \exp(b_0 + b_1 T_0^{-1} + b_2 \ln(T_0) + b_3 T_0) = 6.111536 \text{ hPa}$.

The difference between the Goff-Gratch formula and the Murphy-Koop formula, in percent, is shown in Fig. 2:

⁶this form differs from that of Murphy and Koop (2005) only to present it in a form that is independent of dimensions, except that absolute temperature, conventionally in kelvin, is needed

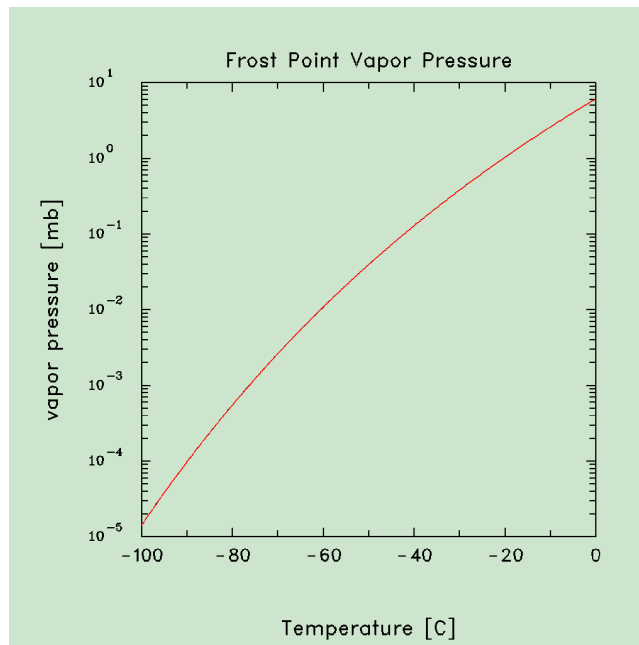


Figure 1: Vapor pressure as a function of frost point from the Murphy and Koop (2005) formula. The Goff-Gratch formula is superimposed but is not distinguishable in this plot.

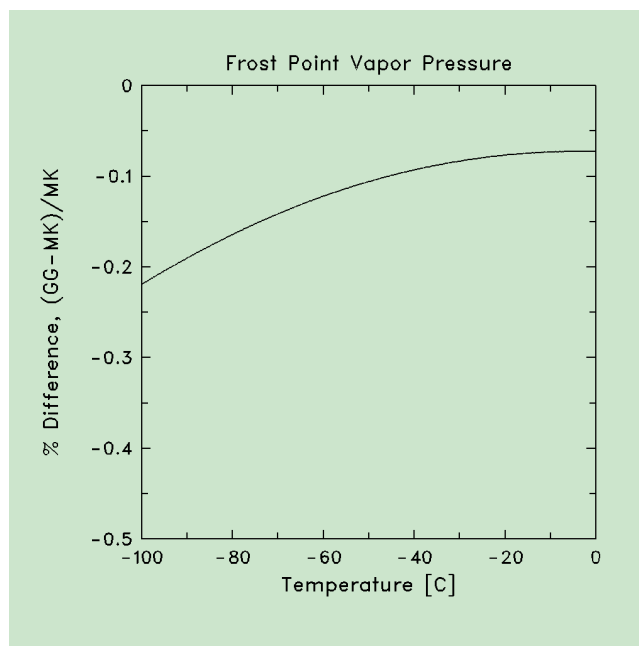


Figure 2: The percentage difference between the Goff-Gratch and Murphy-Koop formulas for frost-point vapor pressure. The plotted value at -100°C indicates that the Murphy-Koop value is about 0.22% higher than the Goff-Gratch value.

Dew Point:

Murphy and Koop (2005) present a single formula that they suggest is valid for the equilibrium vapor pressure over water from 123 K to 332 K, and thus for all temperatures normally present in the atmosphere. The formula is a splice of two fits, using a hyperbolic tangent function to merge the two. The $\tanh()$ function changes from -1 to 1 as the argument changes from large negative to large positive, so it is used to combine the coefficients from the two fits:

$$\ln(e_{s,w}) = d_1 + d_2 \frac{(T_0 - T)}{TT_0} + d_3 \ln\left(\frac{T}{T_0}\right) + d_4(T - T_0) \quad (3)$$

or

$$e_{s,w} = e_0 \exp\left(\left(\alpha - 1\right)e_6 + d_2\left(\frac{T_0 - T}{TT_0}\right) + d_3 \ln\left(\frac{T}{T_0}\right) + d_4(T - T_0)\right) \quad (4)$$

where $T_0=273.15$ K, and if $\alpha = \tanh(e_5(T - T_x))$ with e_5 as in the table below and $T_x = 218.8$ K, $d_i = e_i + \alpha e_{i+5}$, with $e_0 = \exp(e_1 + e_6) = 6.091888$ hPa. The values of e_i are given in the following table:

coefficient	value
e_1	6.564725
e_2	-6763.22 K
e_3	-4.210
e_4	0.000367 K ⁻¹
e_5	0.0415 K ⁻¹
e_6	-0.1525967
e_7	-1331.22 K
e_8	-9.44523
e_9	0.014025 K ⁻¹

Figure 3 shows the vapor pressure as a function of dewpoint from (4). The Goff-Gratch formula is also plotted here, but within the resolution of the plot it is hard to distinguish from the Murphy and Koop equation. However, when the difference is plotted as in Fig. 4, it is evident that the departures at low temperature are significant.

Inverting the Equations:

The Goff-Gratch equation and the Murphy-Koop equation provide vapor pressure as a function of frost point or dewpoint, but it is sometimes useful to be able to calculate the inverse, the frost or dew point given the vapor pressure. For example, this must be done in normal processing to obtain the dewpoint from the measured frostpoint. The equation used for this purpose was given in the first section:

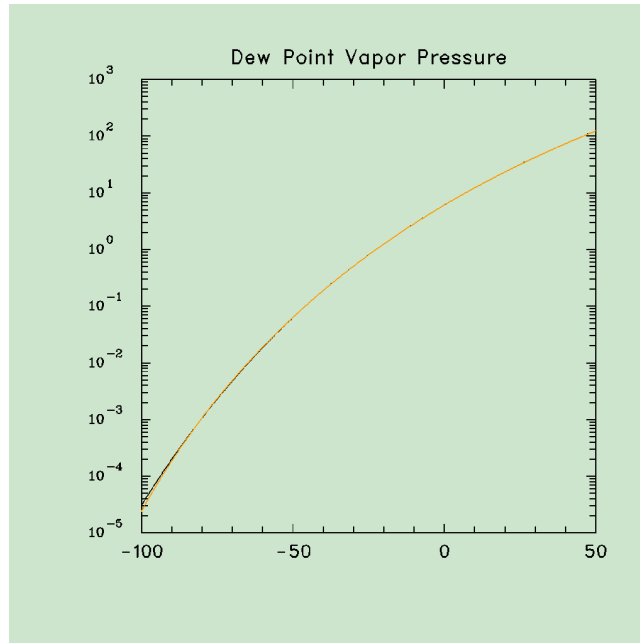


Figure 3: Water vapor pressure as a function of dewpoint for the equation of Murphy and Koop (2005, black line) and also for the Goff-Gratch formula (orange line).

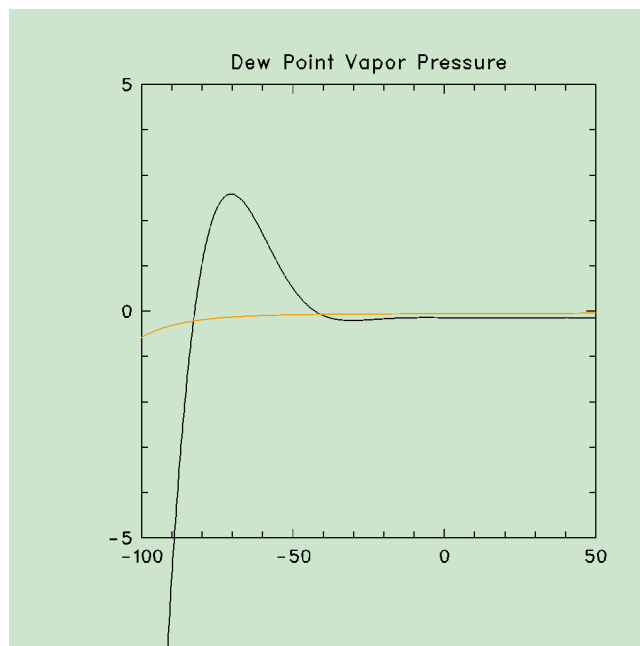


Figure 4: Difference in percent between the Murphy and Koop formula and the Goff-Gratch formula for water vapor pressure as a function of dewpoint. The orange line shows the difference between the Goff (1965) formula and the Goff-Gratch (1946) formula.

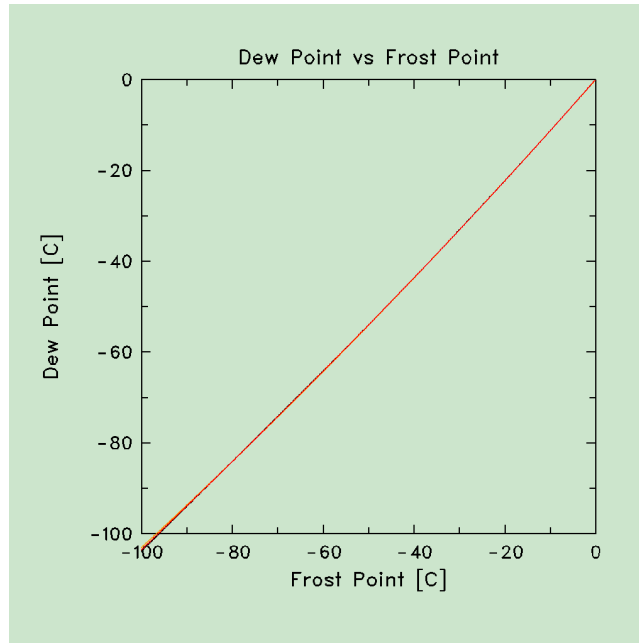


Figure 5: Calculation of frost point from dew point, using the Murphy and Koop (2005) formulas (black line) and using the quadratic formula from nimbus code (orange line).

$$T_d = 0.009109 + T_f(1.134055 + 0.001038T_f) \quad (5)$$

where both T_d and T_f are given in units of °C. To evaluate the accuracy of this formula, the equation from Murphy and Koop for water vapor pressure was inverted numerically to generate a plot of dewpoint as a function of frostpoint, and the result was compared to (5). The result, shown in Figs. 5 and 6, was that (5) produced errors that were typically about 0.2°C for frostpoints near about -60 to -70°C and increasing errors below -90°C that approached 0.8°C. Because of the complexity of the fit at these low frostpoints, it was necessary to use a 4th-order fit to achieve reasonable accuracy, as shown also in Fig. 5. The best-fit coefficients were the following:

$$\begin{aligned} T_d = & 4.953828 \times 10^{-3} + T_f(1.132468 + T_f(8.865794 \times 10^{-4} \\ & + T_f(-5.273161 \times 10^{-6} + T_f(-4.492316 \times 10^{-8})))) \end{aligned} \quad (6)$$

This polynomial is still not as accurate as would be desirable, producing a difference of about 0.2°C at the extreme low temperature of -100°C frost point (the lowest temperature included in the fit). It may be preferable to use a Newton's-method solution of the Murphy-Koop equation because that converges with only a few iterations, typically about 5 for 0.00001°C tolerance in the answer.

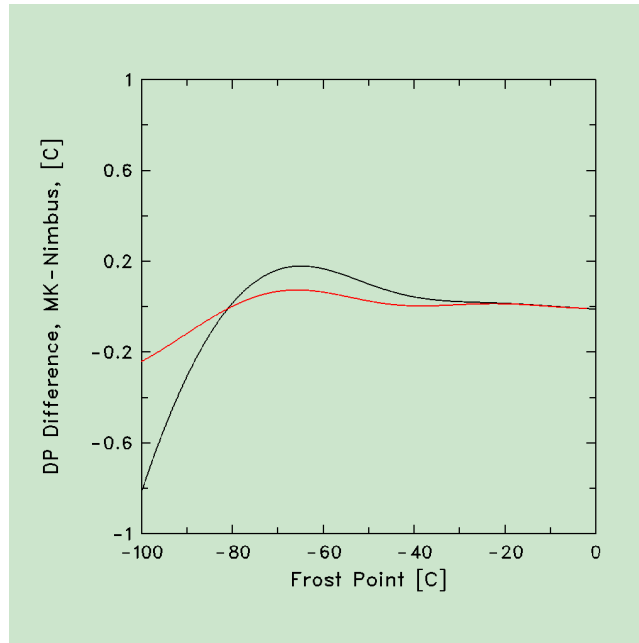


Figure 6: Difference between dewpoint calculated from frost point using the Murphy and Koop (2005) equations vs the nimbus code (black line) or vs the fourth-order polynomial given in the text (orange line).

Recommendations:

1. Replace the Goff-Gratch formulas for vapor pressure in equilibrium over ice or water surfaces with the formulas (2) and (4), respectively. This is not a significant change that would require any reprocessing, but it brings us into line with current best equations, especially in the region that pertains to supercooled water.
2. Replace calculation of the dewpoint from the frostpoint with a Newton's-method solution of the above equations, which provides an accurate solution throughout the applicable temperature ranges, provided that tests demonstrate that the time required for such solution is negligible. (If not, the fourth-order polynomial fit given in the preceding section may be preferable.) This procedure can also be used to find the equivalent dew-point temperature corresponding to other measurements, such as those derived from the measurement of vapor density directly, provided that the results are first converted to a measurement of vapor pressure such as provided in the first step below. The solution procedure is as follows:
 - (a) Given the frost-point temperature T_{FP} , use (2) to find the corresponding vapor pressure, set to "ess" before using the following code examples.
 - (b) Use a Newton's-method (or other numerical) solution to find the dew-point temperature T_{DP} that gives the same vapor pressure:⁷

⁷the following code was used to generate the figures in the preceding section

- i. define a function like the following to define the desired zero for Newton's method. To use this, before the function is called, "ess" should be set to the vapor pressure corresponding to the frost point for which the dewpoint is to be calculated, in units of hPa or mb:⁸

```
float vapMK(float *tc)
{
// this uses the global reference pressure ess, obtained
// from the Murphy and Koop formula for ice vapor pressure
// and set before this function is called
double tk, yp;
const double tz = 273.15;
const double b7=54.842763, b8=-6763.22, b9=-4.210,
             b10=0.000367, b11=0.0415, TR2=218.8, b12=53.878,
             b13=-1331.22, b14=-9.44523, b15=0.014025;
// convert to kelvin
tk = *tc + tz;
yp = exp(b7 + b8 / tk + b9 * log(tk) + b10 * tk
        + tanh(b11*(tk-TR2)) * (b12 + b13 / tk
                               + b14 * log(tk) + b15 * tk))/100.;
yp -= ess;
return(yp);
}
```

- ii. use some code similar to the (decades-old) FORTRAN code in the next box to find the zero of the preceding function:
- iii. use a subroutine call similar to the following C code to find the dewpoint ("td") from the frost point ("tf"):
newtn_(&vapMK, &tf, &eps, &td);
where "const float eps = 0.00001" specifies an (overly strict) accuracy limit on the result, which could be made larger if it proves necessary to limit the number of iterations. The variable "tf" is only passed to the subroutine to provide an initial value for the iteration; the vapor pressure "ess" must be set to correspond to this frost point prior to calling the subroutine. Both "tf" and "td" are in units of °C.

3. Modify the correction for atmospheric pressure, now described in RAF Bulletin 9 Appendix C, to have the form given by (1), duplicated here:

$$f = 1 + 10^{-5} p(4.923 + T(-0.0325 + T(5.84 \times 10^{-5})))$$

where p is the total pressure in hPa or mb and T is the temperature in kelvin. There is a

⁸the equation and coefficients in the following are as given by Murphy and Koop (2005) and differ from those of (4) only as a result of consolidation of coefficients and reformulation to avoid dimensional specificity in the original formula

Algorithm 0.1 ancient FORTRAN example of one way to implement Newton's method

```
      SUBROUTINE NEWTN(FUNC,X0,EPS,XC)
C.....SOLUTION OF EQUATION FUNC=0 BY NEWTON'S METHOD
C
C.....INPUT:
C          FUNC = FUNCTION IN FORM F(X)=0.  EITHER IMPLICIT
C          IN CALLING PROGRAM OR DECLARED EXTERNAL.
C          X0   = STARTING GUESS AT ROOT.
C          EPS  = DESIRED TOLERANCE IN ANSWER.
C.....RESULT:
C          XC   = ROOT OF EQUATION.
      LOOP=1
      XB=X0*1.01
      XA=X0
      DELTA=XB-XA
      FA=FUNC(XA)
1     FB=FUNC(XB)
      FPRIME=(FB-FA)/DELTA
      XC=XB-FB/FPRIME
      DELTA=XC-XB
      XB=XC
      XA=XB
      FA=FB
      IF(LOOP.GT.500) RETURN
      LOOP=LOOP+1
      IF(ABS(DELTA).GT.EPS*0.1) GO TO 1
      RETURN
      END
```

subtlety in application of this formula that should be observed, however. The dewpoint has two definitions that are usually considered identical, but they are not, although both of the following quotes are taken from the AMS Glossary:

- (a) “The temperature to which a given air parcel must be cooled at constant pressure and constant water vapor content in order for saturation to occur.”
- (b) “... the temperature at which the saturation vapor pressure of the parcel is equal to the actual vapor pressure of the contained water vapor.”

The equation for f shows that there is an excess vapor pressure at equilibrium as a result of the total pressure, so a parcel cooled to saturation will condense at a temperature that differs from the saturation vapor pressure as that term is usually understood, i.e., the saturation vapor pressure in the absence of air. Definition (b) is only equivalent to (a) if “the saturation vapor pressure of the parcel” is considered to be pressure-dependent, which I think is not the usual assumption. I suggest that the resolution to this is to consider dewpoint temperature or frostpoint temperature to be the temperature at which the vapor in the parcel⁹ has partial pressure equal to the equilibrium vapor pressure at that temperature but in the absence of air. That leads to a unique correspondence between frost or dew point and vapor pressure, whereas definition (a) above would mean that at a given frost or dew point the vapor pressure would vary depending on the pressure. If we follow this convention, it has consequences for how we use the enhancement factor f :

- (a) Regarding performance of the dew-point hygrometers, we should assume that they measure a frost- or dew-point temperature that *has already been enhanced* by f , so that the measurement should be corrected by adjusting the frost- or dewpoint to be the value that would give equilibrium vapor pressure *in the absence of air*. Suppose the instrument measures a frost-point temperature T'_{FP} . That means that the vapor pressure is *higher* than the equilibrium vapor pressure at T'_{FP} by the factor f , such that $e = e_{s,i}(T_{FP}) = f e_{s,i}(T'_{FP})$, so the true frost-point temperature T_{FP} is higher than T'_{FP} and the measured value should be corrected upward to obtain a true frostpoint in the sense defined above. Two alternatives are the following. (I think the first is most straightforward.)
- i. One can calculate the vapor pressure from the measured frost-point temperature, using (2), and then apply the enhancement factor f to get a value for the vapor pressure, in analogy to what is done now (but using the correct enhancement factor that applies to the ice region). Then use that enhanced value of the vapor pressure to calculate the dewpoint temperature according to the procedure above. This

⁹not “the vapor *contained* in the parcel”: the AMS glossary perpetuates the misconception that the air contains the water vapor, as in the often-mistated claim that warm air “holds” more water vapor than cold air. This is also an argument against using the term “saturation” vapor pressure; the vapor is not “saturating” anything, and it would be better to use the term “equilibrium vapor pressure” instead, although I haven’t followed that convention in this note as consistently as I should

is simpler than the approach of the next paragraph and is equivalent as long as the process is applied to *all* measurements, including those where the measured temperature is above 0°C.

- ii. One can adjust the frost point to be the frost-point temperature that would be measured in the absence of air at the same vapor pressure. The following correction based on linear extrapolation will be adequate:¹⁰

$$\delta T_{FP} = \frac{e_s(T_{FP})(f - 1)}{de_s(T_{FP})/dT_{FP}} \quad (7)$$

- (b) Then, to use that frost-point measurement to determine vapor pressure, one should use the equilibrium vapor-pressure formula (2) without correction, and calculation of the dew-point temperature from that frost-point temperature similarly should not involve any consideration of enhancement factors. This results in the same vapor pressure as that obtained by applying the correction as an enhancement to the vapor pressure, as is now done, but it restores the unique correspondence between frost-point temperature and vapor pressure. The required adjustment can typically amount to 0.5% in vapor pressure or, correspondingly, about 0.07°C difference in dew-point temperature. *The significant change would be that the corrected dewpoint temperature will be that applicable in the absence of air, independent of total pressure, with unique correspondence to vapor pressure.*
- (c) When using humidity measurements from devices that measure water-vapor density directly, those measurements should not have any correction applied for the enhancement factor. After determining the water vapor pressure from the measurement, one should use the procedure described above to invert (4) to obtain an equivalent dewpoint, without any adjustment for enhancement factor. This and the above changes in calculation of the dewpoint will make the measurement equivalent to that obtained from the dew-point hygrometers, but only if the adjustment above is applied to the latter; otherwise, the instruments would be reporting different quantities (as is the case now, because the chilled-mirror devices produce a corrected dewpoint that differs from the dewpoint equivalent to the measured vapor pressure, while the instruments measuring vapor density are translated into equivalent dewpoint that is equivalent to the measured vapor pressure without enhancement).

¹⁰i.e., the frost point measured by the frost-point hygrometer should be corrected by the addition of δT_{FP}