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Background

A quantity often called the equivalent potential temperature is used to represent stability for adiabatic wet processes and to correspond to wet adiabats on thermodynamic diagrams. Potential temperatures are generally defined to correspond to specific entropy (i.e., entropy per mass of dry air) via the relationship $c_{px}d\ln\Theta_x = ds$ where "x" indicates that various kinds of potential temperatures can be defined that satisfy this relationship for different processes. The AMS glossary restricts the term equivalent potential temperature to true adiabatic processes, where any condensed water remains in the parcel, but the term is often used (and has been used in Bulletin 9 Appendix B) to refer instead to the modified pseudo-adiabatic form (sometimes called pseudo-equivalent potential temperature or pseudo-adiabatic equivalent potential temperature) in which the specific heat capacity of any condensed water is neglected in the adiabatic process. This is equivalent to assuming that any condensed water falls from or is otherwise removed from the parcel as it condenses. In this memo, I will refer to the former potential temperature as the wet-equivalent potential temperature (symbol Θ_q) and the latter as the pseudo-adiabatic equivalent potential temperature (symbol Θ_p).

For Θ_p, a problem that arises is that the latent heat L_v must vary with temperature T, even if the specific heats are constant, as specified by the Kirchhoff equation: $dL_V = (c_{pv} - c_w)dT$ where c_{pv} is the specific heat of water vapor at constant pressure, c_w is the specific heat of liquid water. Some generalized equations have been developed that treat this variation in various ways, mostly by using an adjusted value of L_V that produces the least compromise in accuracy. See esp. Bolton (1980) and Davies-Jones (2009). Emanuel (1994) and the preceding two references present derivations of the pseudo-adiabatic equivalent potential temperature.

Present Processing Code

The code from subroutine thetae.c includes the following code (where atx is converted to units of kelvin earlier in the code):

```
    tlcl = (2840.0 / (3.5 * log((double)atx) - log((double)edpc) - 4.805)) + 55.0;
        ...
    theta = atx * pow((double)1000.0 / psxc, (double)0.28571);
    exparg = ((3.376 / tlcl) - 0.00254) * (mr * (1.0 + (0.00081 * mr)));
        ...
    PutSample(varp, theta * exp((double)exparg));
```
This is based on equation (38) from Bolton (1980):

$$\Theta_E = \Theta\exp\left\{\left(\frac{3.376}{T_L} - 0.00254\right)r(1 + 0.81\times10^{-3}r)\right\} \qquad (1)$$

where

$$T_L = \frac{2840}{3.5\ln T_K - \ln e - 4.805} + 55 \tag{2}$$

is the temperature at the LCL (Bolton 1980, Eq. (21)).

Reasons For Proposing Changes

1. The equation selected from Bolton (1980) is the less accurate of several alternatives presented there. Davies-Jones (2009) has pointed out that the form given as equation (39) in Bolton is more accurate, and Bolton also notes that. His more accurate formula is:

$$\Theta_p = \Theta_{DL} \exp\left\{ \left(\frac{3.036}{T_L} - 0.00178 \right) r \left(1 + 0.448 \times 10^{-3} r \right) \right\} \tag{3}$$

   where

$$\Theta_{DL} = T_k \left(\frac{1000}{p_d} \right)^{0.2854} \left(\frac{T_K}{T_L} \right)^{0.28 \times 10^{-3} r} \tag{4}$$

   is the potential temperature of dry air at the lifting condensation level (LCL) and T_L is the temperature at the LCL as given by (2). Equation (3 takes into account the effect of humidity on the ratio of specific heats of the water-saturated air parcel. This form appears to be a better choice than the one now in use.[1]

2. The Bolton fits were based on a representation of the equilibrium water vapor pressure that is different from the one now entering use in the RAF processing code. Bolton determined a fit to the data of Wexler (1976), all of which were for temperature higher than 0°C. He used extrapolation of the measurements to lower temperature, but did not test his new fit for temperatures below -35°C. Because there are now more reliable representations of the water vapor pressure (esp. Murphy and Koop 2005), it is important to check if the Bolton formula (Bolton, 1980, equation (10)) is an adequate representation of equivalent potential temperatures calculated with the new data.

3. More significantly, the Murphy and Koop formula is based on estimates of the specific heat of liquid water in the supercooled region that vary significantly, while previous analyses like those of Bolton and of Davies-Jones (described in the next paragraph) have used constant specific heats. Some justification for use of whatever formula is used for processing is therefore needed.

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[1] Because Bolton used fits to adjust coefficients in this formula and in (1), coefficients should be adjusted to modern values only with care. Davies-Jones (2009) has provided updated coefficients based on a similar but more extensive procedure.

4. Davies-Jones (2009) presents a new formula that appears to be slightly more accurate than the formulas of Bolton (1980), and he also optimized a large set of candidate expressions by adjusting the coefficients (including those of Bolton) to match results from exact integrations of the entropy formulas.[2] His new formula (Davies-Jones, 2009, Eq. (6.5)) is

$$\Theta_p^{[DJ]} = \Theta_{DL} \exp \left\{ \frac{(L_0^* - L_1^*(T_L - T_0) + K_2 r) r}{c_{pd} T_L} \right\} \qquad (5)$$

where Θ_{DL} is as defined by (4), $L_0^* = 2.56313 \times 10^6 J kg^{-1}$, $L_1^* = 1754$ J kg^{-1}K^{-1}, and $K_2 = 1.137 \times 10^6$ J kg^{-1}. The asterisks on L_0^* and L_1^* indicate that these are the result of his optimization procedure and therefore depart slightly from the coefficients that would provide the best match to the latent heat of vaporization.

5. The name of the variable "THETAE" should be changed to be consistent with usage recommendations of the AMS Glossary.

6. It may be useful to include a new variable, the wet-equivalent potential temperature Θ_q, in the data files. This is easier to calculate and less controversial than Θ_p, and it enters analyses that have become widely used like the analyses of Paluch (1978).

Perhaps arguing against change is that, as long as we state clearly what the basis for the calculation is, users are always able to calculate a different variable of their choice from the basic measurements that are in the data set, so the variable in the data files does not constrain users. It may be preferable to retain the current equation or make small changes to represent the best values in the Bolton (1980) paper, rather than make a change, because use of the Bolton formulas has become the common convention. However, I still recommend a change to either the higher-accuracy version from Bolton (1980) or, preferably, to the Davies-Jones (2009) formula. This makes our data files consistent with what appears to be the most accurate equation available, and it moves closer to the goal of producing a value that is conserved during pseudo-adiabatic processes.

Analysis

The desired relationship between entropy and Θ_q is $ds = c_{pt} d \ln \Theta_q$ where $c_{pt} = c_{pd} + r_t c_w$. The integral of this relationship involves an integration constant, which can be selected so that s is relative to a state with $T = 1$ K, $r = 0$, $r_w = 0$, and $p_d = p_0$ where p_0 is the reference pressure, 1000 hPa. In the case where the specific heats are constant (but L_V still varies in accord with the Kirchhoff equation), the equation for the wet-equivalent potential temperature is

$$\Theta_q = T \left(\frac{p_0}{p_d} \right)^{R_d/c_{pt}} \exp \left\{ \frac{L_v r}{c_{pt} T} \right\} \left(\frac{e}{e_s(T)} \right)^{-rRw/c_{pt}} \qquad (6)$$

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[2]However, he has also used an approximate equation from Bolton (1980) to represent the vapor pressure.

where the last term, often not included, arises in case of a subsaturated parcel (below its LCL). (See the derivation in Emanuel, 1994, leading to his equation (4.5.11).) This equation arises from expressing the entropy of the parcel in terms of its temperature, pressure, and mixing ratio, and then rearranging the result into an integrable form.

In the case of Θ_p, the result is not integrable even with constant specific heats because, with neglect of the heat capacity of the water carried with the parcel, the replacement for c_{pt} is $c_{pt}^{\dagger} = c_{pd} + rc_w$ and this depends on r, unlike c_{pt} which is a constant. This is the reason that various approximate formulas have been developed to represent Θ_p, including those of Bolton (1980) and Davies-Jones (2009).

Despite this advantage of Θ_q, it has the disadvantage that it cannot be plotted on a thermodynamic diagram because it does not depend uniquely on T and p as do the conventional definition of potential temperature (Θ) and pseudo-adiabatic equivalent potential temperature (which is a unique function of T and p along saturated adiabats because the condensed water is removed so the dependence on history, which would lead to variable liquid water content in the case of Θ_q, is lost).

The question to be addressed here is this: To what extent do relationships based on various equations for Θ_p and Θ_q depart from the representation of the entropy that arises from direct integration of the expression for entropy relative to the reference state? Some of the mathematical development of this argument is included in the long form of this note. This question can be addressed by evaluating the extent to which constant values of Θ_p or Θ_q represent true pseudoadiabats or wet adiabats during vertical motion of air parcels. Davies-Jones (2009) has addressed this question for the Bolton formulas, a new alternative he proposed, and some others. However, two considerations not discussed there are relevant to RAF applications:

- What is the effect of introduction of the Murphy and Koop (2005) representation of equilibrium water vapor pressure? This will result in small shifts in results but should not affect the analysis of accuracy as presented by Davies-Jones (2009) because the formulas have vapor pressure as an input. The Davies-Jones analysis adjusts of coefficients in the formulas to compensate for factors like the variation in latent heat with temperature, and those coefficients have been minimized by comparison to numerical integrations that use old representations of vapor pressure. However, this does not seem likely to have much effect on the results because the vapor-pressure formula used is close to the revised form presented by Murphy and Koop (2005) and because the vapor pressure would enter both the parametrized formula and the exact integration in compensating ways.

- What is the effect of temperature dependence of the specific heats, esp. that of supercooled water? The temperature dependence of the specific heats is neglected, both in the parametrized formulas and in the exact integration as done by Davies-Jones, Bolton, and others. However, the vapor-pressure formulas offered by Murphy and Koop (2005) are based on a representation of the specific heat of supercooled water that has significant variation, of order 50% overall. This applies to the wet-equivalent potential temperature as well as the pseudo-adiabatic equivalent potential temperature.

One approach to both questions is to integrate $dT = (dT/dp_d)dp_d$ using the exact relationship for entropy and compare the result to that obtained from the formulas that were obtained with constant specific heats. For example, consider a case where the temperature and dry-air pressure are T_1 and $p_{d,1}$ and the parcel is saturated. One can obtain the temperature at a low pressure $p_{d,2}$ (e.g., 100 hPa) by evaluating the appropriate formula for Θ_q or Θ_p, then inverting that formula to obtain the temperature at $p_{d,2}$ that gives the same corresponding equivalent potential temperature. For comparison, one can integrate to obtain the same temperature. If the temperature dependence of the specific heats is included in the latter integration, the difference between results will provide a measure of the error in equivalent potential temperature obtained from the formula used for its evaluation.

To do this, the temperature dependence of the specific heats must be represented. The accompanying long-form note contains an Appendix that specifies the data available and used for the integrations. The most important variation is that of the specific heat of liquid water (including in the supercooled region), which varies quite significantly (more than 50%) in the supercooled region. Because the water vapor pressure becomes quite low for substantial supercooling, it is not clear that even this very large variation has a significant effect, but this is likely to be the dominant term causing a departure from constant-c_p formulas. The specific heat of dry air, in contrast, varies little (less than 0.1% from -50°C to +40°C, and less than 0.4% from -100 to +60°C), so that variation will be neglected here. The specific heat of water vapor does not enter the formulas for pseudo-adiabatic or wet equivalent potential temperature, but it does enter indirectly through the Kirchhoff equation, which relates the temperature dependence of L_v to the difference between the specific heats of water vapor and liquid water. At $p_{d,2} = 100$ hPa, inversion of these formulas give the respective temperatures 178.69 K and 175.66 K. For comparison, integrations from point 1 to point 2 using direct integration as developed in the accompanying long-form note or the analog with $c_{pt}^{\dagger} = c_{pd} + rc_w$ give the respective values 178.71 K and 175.69 K, both quite close to the values obtained by the respective equations.

The following table gives these and a few more values, where T_q and T_p are the temperatures determined at the final pressure p_2 from inversion of the formulas for Θ_q and Θ_p, and the corresponding primed quantities are the temperatures determined by numerical integration that incorporates the variation in specific heat.:

T [°C]	p [hPa]	final p_2 [hPa]	$T_q[K]$	$T_q'[K]$	$T_p[K]$	$T_p'[K]$
25	850	100	206.50	207.69	200.73	200.76
15	750	100	189.34	189.73	185.39	185.42
10	750	100	178.69	178.71	175.66	175.69
0	700	100	167.05	166.90	165.39	165.41
-10	600	100	163.54	163.44	162.68	162.70
25	850	300	222.59	222.69	222.27	222.29
10	750	300	239.43	239.46	238.52	238.51
0	700	300	226.46	226.59	225.82	225.84

Although the evaluation is not exhaustive, it appears to support these conclusions:

1. Comparison of the last two columns suggests that the formula (5) represents the pseudo-adiabats with good accuracy, even when they are calculated using the strong variations in the specific heat of liquid water estimated by Murphy and Koop (2005) and using the Murphy and Koop vapor pressures.

2. Even for the reversible adiabatic equation (6), there is only minor deviation from true adiabats when the temperature variation of the specific heats is represented accurately. The variations from the temperature on a true wet adiabat are only a few tenths degree in most cases, but over 1 K in the extreme case. One might expect more variation, because high liquid water content can be carried upward where the variation in specific heat of liquid water can affect the answer. These are unrealistic situations, however, because high liquid water content cannot exist at temperatures as low as the extremes of this integration.

One additional issue is the representation in cases where the parcel is unsaturated. Equation (5) represents the pseudo-adiabatic equivalent potential temperature in terms that involve the saturation temperature, the temperature at the LCL. This is now done using (2) from Bolton (1980), but if the specific heats are functions of temperature and vapor pressure is changed to the representation of Murphy and Koop (2005), it is not clear that this choice remains valid.

Alternately, one can determine the temperature of the lifted parcel at the LCL from the conserved values of mixing ratio and moist potential temperature, iteratively evaluated for the temperature that gives the equilibrium vapor pressure. To evaluate how well the Bolton formula for T_L represents exact values, a set of calculations were performed where the LCL was determined by this iterative procedure. More detail regarding the procedure is included in the long-form note. A short list of checks, shown in the following table, suggested that the Bolton formula (2) for T_L performs well, giving values within 0.05 K of those determined by the numerical solution. Because this is a published equation in common use, there does not appear to be any need for a change.

Temperature [°C]	Pressure [hPa]	RH [%]	(2) – Bolton	Numerical
20	850	50	280.074	280.067
25	900	30	275.42	275.43
25	900	20	290.94	290.92
10	700	80	279.14	279.14
10	700	50	271.12	271.24
10	700	10	247.54	247.58
0	600	80	269.45	269.48
0	600	40	258.79	258.84
0	600	20	249.13	249.18

Recommendations:

1. Change to (5), and change the variable name to "pseudo-adiabatic equivalent potential temperature". Use (2) to determine the saturation temperature T_L. (There will need to be some

protection against the relative humidity exceeding 100%; if it does, set it to 100% for this calculation.)

2. Add a new variable "wet equivalent potential temperature" and use (6) for its evaluation. A caution should be included to warn users that there may be inaccuracies in Θ_q of a few tenths kelvin that arise from variation and uncertainty in the specific heat of supercooled water.

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