On Formulas for Equivalent Potential Temperature

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ABSTRACT

Several new formulas for pseudoadiabatic equivalent potential temperature (EPT) are devised and compared to previous ones. The maximum errors of all the formulas are determined from calculations on a dense grid of points in the region of a thermodynamic diagram defined by wet-bulb potential temperature $\leq 32°C$ (EPT ≤ 400 K) and pressure between 100 and 1050 mb. One of the new formulas has an accuracy of 0.015 K in the specified region. Finding the imitation first law of thermodynamics that they satisfy approximately reveals how the formulas work.

1. Introduction

There are several formulas for equivalent potential temperature (EPT) in the literature (Bolton 1980; Bryan 2008). Rossby (1932) devised the first such formula by dropping an intractable term from the equation governing pseudoadiabatic water-saturation processes. This term is part of the entropy of water vapor. Its omission is equivalent to setting the specific heat of water to zero. Owing to the missing entropy, the Rossby formula underestimates the EPT by several degrees in very warm and moist environments. By using an optimized constant latent heat instead of the actual one, which is a linear function of temperature, Bryan (2008) obtained a simple formula that is accurate to about half a degree. His formula is associated with a simple version of the first law of thermodynamics, which is useful in some theoretical studies. Except at very cold temperatures where latent heat release is small, Bryan's constant latent heat is larger than the actual one. The upward adjustment in latent heat compensates to a large extent for the missing term. Bolton's (1980) modification of the Betts and Dugan (1973) formula is similar to Bryan's formula, and is also associated with a constant latent heat (Davies-Jones 2008).

The most accurate formula to date is from Bolton (1980). It computes EPT to accuracy, relative to numerical solutions of the governing equation, better than 0.02 K. Note that accuracies quoted in the literature are based on a limited number of calculations (e.g., Bolton's Table 3 and Bryan's Table 1). Bolton's formula has three adjustable parameters and is hard to interpret physically.

In this paper, the gap between Bryan's formula with one adjustable parameter and Bolton's very accurate formula with three is bridged by constructing formulas that have two degrees of freedom and intermediate accuracies. These new formulas are obtained by optimally adjusting the line in a graph of latent heat versus temperature instead of constraining it to have zero slope. Also, understanding of how the formulas work is gained by working backward from the formulas to an imitation first law of thermodynamics that they satisfy. This procedure identifies the adjustments needed to compensate for setting the specific heat of water to zero. Bolton's formula is not amenable to this approach so a very similar, but more manageable formula with the same accuracy is devised. Last, maximum errors of each formula are determined more systematically than previously by calculating EPT at 1209 points in a grid covering a wide area of a thermodynamic diagram.

2. EPT formulas

As pointed out by Davies-Jones (2008), almost all of the formulas for the EPT θ_E of an air parcel have the following form:

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$$\theta_E^* = \Theta \exp\left[\frac{L_0^* - L_1^*(T_L - C)}{c_{pd}T_L} r(1 + k_2 r)\right], \quad (2.1)$$

where L_0^* (>0), L_1^* (≥ 0), and k_2 (≥ 0) are constants, θ_E^* is the estimate of θ_E, T_L is the temperature at the lifting condensation level (LCL), and r is the mixing ratio. All symbols and a few useful relationships are listed in the appendix. The quantity Θ is either the potential temperature θ of moist air, which is conserved in unsaturated isentropic motion, or the potential temperature of dry air at the LCL, θ_{DL}. These formulas apply to all levels because T_L, θ_{DL}, r, and e can be replaced by T_K, θ_D, $r_s(T_K, p)$, and $e_s(T_K)$, respectively, above the LCL. Associated with (2.1) is the approximate equation for pseudoadiabatic ascent:

$$c_{pd}d\ln\theta_E^* = c_{pd}d\ln\Theta + d\left[\frac{L_0^* - L_1^*(T_L - C)}{T_L} r(1 + k_2 r)\right]$$
$$= 0, \qquad (2.2)$$

and the adjusted entropy:

$$s_p^* \equiv c_{pd}\ln\theta_E^* = c_{pd}\ln\Theta + \frac{L_0^* - L_1^*(T_L - C)}{T_L}r(1 + k_2 r). \qquad (2.3)$$

The first and least accurate formula for EPT is the one devised by Rossby:

$$\theta_E' = \theta_{DL}\exp\left[\frac{L(T_L)r}{c_{pd}T_L}\right], \qquad (2.4)$$

where θ_E' denotes the Rossby EPT and L is the actual latent heat. It underestimates the actual EPT by up to 5° in extremely humid air masses because it uses the actual latent heat $L \equiv L_0 - L_1(T_L - C)$ and ignores the term involving the specific heat of water in the entropy formulation. However, it sufficed for its original purpose, the identification of air masses. Because the omitted entropy term $c_w r_s\, d\ln T_K$ is positive, θ_E' is always an underestimate of θ_E. The Rossby formula has no parameter that can be adjusted to compensate for the missing entropy. A further approximation consists of replacing θ_{DL} by θ (Iribarne and Godson 1973, p. 122).

When $k_2 = 0$, comparison of (2.1) and (2.4) shows that we can regard $L^* \equiv L_0^* - L_1^*(T_L - C)$ as a surrogate for L. We can obtain more accurate formulas for EPT by adjusting the two latent heat coefficients. Generally, formulas with more degrees of freedom (the number of independent parameters that are varied to obtain a best

fit to data) match the data more accurately. The third degree of freedom, k_2, is needed for a very accurate fit.

Using this approach Betts and Dugan (1973), Simpson (1978), Bolton (1980), and Bryan (2008) have devised formulas that are similar to (2.4), but that match the exact pseudoadiabats far better. Since the equations in Bolton's paper are referenced many times, we will preface his equations numbers with a ''B.'' Similarly, Bryan's (2008) equations are prefaced with ''Br.'' We do not consider Simpson's formula [(B33) after Bolton's modification] further because it is less accurate than (B38) and (B39), has a more cumbersome form, assumes that θ_D is conserved during adiabatic ascent to the LCL, and is not easily associated with an imitation first law of thermodynamics. Bolton simplified Betts and Dugan's (1973) formula to

$$\theta_E = \theta\exp\left(\frac{L_0^*r}{c_{pd}T_L}\right), \quad L_0^* = 2.690 \times 10^6 \text{ J kg}^{-1},$$
$$L_1^* = 0, \qquad (2.5)$$

which is equivalent to (B35). This has one degree of freedom, L_0^*, an optimum constant value of latent heat. Bryan's (2008) formula (Br13) similarly has one degree of freedom. It has the following form:

$$\theta_E = \theta_D \mathcal{H}^{-R_v r/c_{pd}}\exp\left(\frac{L^*r}{c_{pd}T_K}\right), \qquad (2.6)$$

with $L^* = L_0^* = 2.555 \times 10^6$ J kg^{-1}. Here, the relative humidity $\mathcal{H}$ has been introduced to avoid having to compute T_L, and θ_D is used instead of θ.

Bolton's two new formulas, (B38) and (B39), are the most accurate to date. They have the form (2.1) with $k_2 \neq 0$ so they both contain a r^2 term. The difference between them is the use of θ_{DL} in (B39) and θ in the less precise (B38). Although (B38) ostensibly has three degrees of freedom, it in fact has only two because L^* is proportional to L (i.e., L_0^* and L_1^* are not varied independently). Equation (B39) does have three degrees of freedom, and this seems to be the number required for an estimate with maximum error (relative to the results of numerical integration of the differential equation governing pseudoadiabatic ascent) to within 0.03 K. The actual error is around 0.2 K, owing mainly to the specific heat at constant pressure for dry air, assumed to be a constant, varying slightly with temperature and pressure. The corresponding error in pseudo-wet-bulb temperature is less than 0.2 K (Davies-Jones 2008).

The third-order term, $-k_2 L_1^*(T_L - C)r^2$, in (2.1) is much smaller in magnitude than the term $k_2 L_0^* r^2$. When this term is neglected, (2.1) simplifies to

$$\theta_E^* = \Theta \exp\left\{\frac{[L_0^* - L_1^*(T_L - C)]r + K_2 r^2}{c_{pd} T_L}\right\}, \quad (2.7)$$

where $K_2 (\approx k_2 L_0^*)$ is a constant. A formula of this form that is as accurate as (B39) is developed later. Note that all the formulas with $k_2 = 0$ are included in this form.

3. The formulas' imitation first law of thermodynamics

In many cloud models, simplified versions of the first law of thermodynamics are used (Wilhelmson 1977). Only some of these are exact differentials for pseudoadiabatic processes and so have exact corresponding analytical formulas for EPT. On the other hand, the approximation to the entropy form of the first law (Holton 1992, p. 51) that corresponds to an analytical approximate formula for EPT can always be found by differentiating the formula as in (2.1) and (2.2).

For use in theoretical studies, Bryan (2008) found an EPT formula that is associated with a simplified version of the first law. Here, we work backward from the entropy formulation to find an imitation first law that the formulas satisfy with the purpose of understanding how the formulas work. As is customary, we neglect the ice phase, assume that the phases of water are in equilibrium (so that there is no supersaturation) and that the volume of any liquid water in the parcel is negligible, and consider the two extreme cases of adiabatic ascent of air that is saturated with respect to a plane surface of water (Bryan 2008). In the first extreme case, the liquid water remains in the parcel and the total water mixing ratio, $Q \equiv r + r_w$, is constant. This is a reversible process (Saunders 1957) and the liquid water content is said to be adiabatic. The second case is the pseudoadiabatic process where condensate falls out of the parcel immediately after it forms. Normally, the liquid water content in clouds lies between the two extremes (Wilhelmson 1977) although occasionally it may exceed the adiabatic value.

For the reversible process, the differential equation governing entropy has the exact integral:

$$s_r = c_{pd} \ln\theta_D + rc_w \ln T_K - R_v r \ln\mathcal{H} + L(T_K)r/T_K$$
$$+ r_w c_w \ln T_K \quad (3.1)$$

[Emanuel 1994, Eq. (4.5.9)]. After multiplying the differential form of (3.1) by T_K and using (B23), the ideal gas laws for dry air and vapor, and the Clausius–Clapeyron equation:

$$\frac{L dT_K}{T_K^2} = R_v d \ln e_s, \quad (3.2)$$

we find that

$$T_K ds_r = dh - \alpha_d \, dp = 0, \quad (3.3)$$

where $h \equiv (c_{pd} + Qc_w)T_K + Lr$ is the specific moist (reversible) enthalpy (Emanuel 1994, p. 118). By applying Kirchoff's equation:

$$\frac{dL}{dT_K} = c_{pv} - c_w, \quad (3.4)$$

we obtain the first law

$$T_K \, ds_r = (c_{pd} + rc_{pv} + r_w c_w) \, dT_K - \alpha_d \, dp + L \, dr = 0. \quad (3.5)$$

In the pseudoadiabatic process, the liquid water is removed immediately from the parcel ($r_w = 0$) so total water is no longer conserved. The entropy, EPT and first law are now

$$s_p = c_{pd} \ln\theta_D + c_w \int_{\tau=T_0}^{T_K} Y(\tau) \, d\tau + L(T_K)Y(T_K)$$
$$- R_v r \ln\mathcal{H}, \quad (3.6)$$

$$\theta_E = \theta_D \mathcal{H}^{-R_v r/c_{pd}} \exp\left\{\frac{Y(T_K)}{c_{pd}}\left[L(T_K) + \frac{c_w}{Y(T_K)}\right.\right.$$
$$\left.\left. \times \int_{T_0}^{T_K} Y(\tau) \, d\tau\right]\right\}, \quad (3.7)$$

and

$$T_K \, ds_p = (c_{pd} + rc_{pv}) \, dT_K - \alpha_d \, dp + L(T_K) \, dr = 0, \quad (3.8)$$

where $Y(T_K) \equiv r/T_K$ and T_0 is a very cold temperature where the integrand is effectively zero. The integral term in (3.6) is part of the entropy of water vapor. It is not zero because, in the pseudoadiabatic process, water condenses and then is removed instantly, along with its entropy, as the parcel is rising and cooling, not while it is maintained at a constant temperature (Bolton 1980).

The exact formula for θ_E is (3.7), but it is not useful because it contains an integral. Since the integral is not an exact differential, the integration has to be performed numerically along a pseudoadiabat. This is tantamount to generating pseudoadiabats by stepwise numerical integration so nothing has been gained. Useful formulas

for s_p and θ_E that depend only on the initial and final states of the parcel have either ignored this term or replaced it implicitly by a compensating term that is an exact differential. Alternatively, we can set $c_w = 0$ and explicitly adjust some other coefficients to minimize the resulting error. This is the approach adopted here.

In fact, the formulas that have the simplified form in (2.7) may all be obtained by setting $c_w = 0$, which eliminates the computationally expensive integral term, and adjusting L (and K_2 if nonzero) to minimize error. In other words, $c_w \to c_w^* = 0$, $L_0 \to L_0^*$ and $L_1 \to L_1^*$ where the superscript asterisk denotes that the coefficients have been adjusted. This gives us the estimate

$$\theta_E^* = \theta_D \mathcal{H}^{-R_v r/c_{pd}} \exp\left[\frac{L^*(T_K)r + K_2 r^2}{c_{pd}T_K}\right]. \quad (3.9a)$$

The EPT estimate, θ_E^*, should be conserved below the LCL. We can ensure this by integrating the entropy equation just for the pseudoadiabatic part of the ascent, and evaluating the constant of integration at the LCL. This yields

$$\theta_E^* = \theta_{DL} \exp\left[\frac{L^*(T_L)r_s(T_L) + K_2 r_s^2}{c_{pd}T_L}\right]. \quad (3.9b)$$

We now find that an imitation first law that corresponds to (3.9). In turns out that in the temperature range $-47° < T_K - C \le 32°C$, $1 < L^*/L < 1.06$ for the formulas with $\Theta = \theta_D$, so to a quite good approximation we can use (3.2) with L^* instead of L. From (3.9a) and the modified (3.2), we obtain

$$0 = T_K ds_p^* = c_{pd}T_K - \alpha_d\, dp + d(L^* r)\, dh^*$$
$$+ K_2 T_K d(r^2/T_K). \quad (3.10)$$

Since r^2 varies much more rapidly than T_K at high mixing ratios where the last term is important, we can approximate (3.10) by

$$T_K ds_p^* = dh^* - \alpha_d\, dp = 0, \quad (3.11)$$

where

$$h^* = c_{pd}T_K + L^*(T_K)r + K_2 r^2 \quad (3.12)$$

is an enthalpy that exists in this simple form because $c_w^* = 0$. Expanding (3.12) gives us the following "first law":

$$T_K ds_p^* = (c_{pd} - L_1^* r)\, dT_K + [L_0^* - L_1^*(T_K - C)]\, dr$$
$$+ K_2 d(r^2) - \alpha_d\, dp = 0. \quad (3.13)$$

If we assume Kirchoff's Eq. (3.4) for the adjusted parameters, then we can define an adjusted specific heat of water vapor, $c_{pv}^* = -L_1^*$ and (3.13) becomes

$$T_K ds_p^* = (c_{pd} + rc_{pv}^*)\, dT_K - \alpha_d\, dp + L^*(T_K)\, dr$$
$$+ K_2 d(r^2) = 0. \quad (3.14)$$

Bryan (2008) set $L_1^* = 0$ (and $K_2 = 0$). Then, (3.6), (3.7), and (3.9) reduce to (Br11), (Br13), and (Br10), respectively, and the enthalpy becomes $h^* = c_{pd}T_K + L_0^* r$.

We can see how the formulas work by comparing (3.8) and (3.14). The adjustment of the specific heat of water to zero and Kirchoff's equation makes the specific heat of water vapor negative (or zero if $L_1^* = 0$). Thus, the specific heat of moist air is reduced artificially. From a first-law viewpoint, an artificial increase in latent heat, $(L^* - L)\, dr$, is required to compensate for the decrease in specific heat. The small r^2 term is extra compensation needed for very accurate calculations of very warm EPTs. From an entropy viewpoint, the entropy increase associated with the increase in latent heat is needed to compensate the entropy of water vapor for the part that is missing.

Which of the forms (3.9a) or (3.9b) is preferable? Equation (3.9a) has the advantage that it does not require computation of temperature at the LCL. But, unlike (3.9b), it does not conserve θ_E below the LCL (Bryan 2008). Thus, a disadvantage of (3.9a) is the introduction of additional error below the LCL as shown below. Since r is constant below the LCL, the integrand in (3.7) has an antiderivative and so (3.7) becomes

$$\theta_E = \theta_D \mathcal{H}^{-R_v r/c_{pd}} \exp\left\{\frac{r}{c_{pd}}\left[\frac{L(T_K)}{T_K} + c_w \ln\frac{T_K}{T_1}\right]\right\}, \quad (3.15)$$

where T_1 is an arbitrary constant of integration. Thus, by conservation of θ_E and (3.15), θ_{DL} and θ_D are related by

$$\theta_{DL} = \theta_D \mathcal{H}^{-R_v r/c_{pd}} \exp\left\{\frac{r}{c_{pd}}\left[\frac{L(T_K)}{T_K} - \frac{L(T_L)}{T_L}\right.\right.$$
$$\left.\left. + c_w \ln\frac{T_K}{T_L}\right]\right\}. \quad (3.16)$$

Substituting for θ_{DL} in (3.9b) gives us

$$\theta_E^* = \theta_D \mathcal{H}^{-R_v r/c_{pd}} \exp\left\{\frac{r}{c_{pd}}\left[\frac{L^*(T_K)}{T_K} + \frac{K_2 r}{T_K}\right.\right.$$
$$\left.\left. - f(T_K) + f(T_L)\right]\right\}, \quad (3.17)$$

where

$$f(\tau) \equiv \frac{L^*(\tau) - L(\tau)}{\tau} - c_w \ln \tau + \frac{K_2 r}{\tau}. \quad (3.18)$$

So (3.9b) implies (3.17), not (3.9a). Although we can apply a correction factor to (3.9a) [to obtain (3.17)], this involves T_L, so we might as well use (3.9b) in the first place.

Using $\Theta = \theta$ instead of θ_{DL} is less expensive computationally, but also leads to more approximation. Bolton states "For most purposes (B38) is probably to be preferred, since it makes use of θ. As a basis for very accurate work, however, (B39) with θ_{DL} given by (B24) is suggested." However, the author prefers using formulas that use θ_{DL} instead of θ for the following reasons. First note that from (B4), (B5), (B7), (B24), and the ideal gas laws for moist and dry air, θ_D, and its value at the LCL, θ_{DL}, are related to θ by

$$\theta_D = \theta \left[\left(\frac{\theta}{T_K} \right)^{0.28r} \left(1 + \frac{r}{\varepsilon} \right)^{\kappa_d} \right],$$

$$\theta_{DL} = \theta \left[\left(\frac{\theta}{T_L} \right)^{0.28r} \left(1 + \frac{r}{\varepsilon} \right)^{\kappa_d} \right]. \quad (3.19)$$

Thus, the extra work involved in computing θ_D or θ_{DL} is relatively minor, and simply replacing θ_D with θ in the exact Eq. (3.7) introduces error by tacitly setting the above quantities in square brackets to 1. Since $\theta < \theta_D$, the adjustment to latent heat has to be larger when $\Theta = \theta$.

4. Approach for devising new formulas

The approach is to minimize the difference between the true specific pseudoentropy and the one associated with a given formula. From (3.6) and (3.9a) this difference for a saturated parcel is

$$s_p^* - s_p = Y(T_K, \theta_E) \left\{ \left[L^*(T_K) + K_2 r_s - L(T_K) - \frac{c_w}{Y(T_K, \theta_E)} \int_{T_0}^{T_K} Y(\tau, \theta_E) \, d\tau \right] \right\}, \quad (4.1)$$

for $\Theta = \theta_D$. [When $\Theta = \theta$, the term $c_{pd} \ln(\theta/\theta_D)$ is added to the right side.] Here, $Y(T_K, \theta_E) \equiv r_s(T_K, \theta_E)/T_K$. To compensate for the omission of the c_w term in (3.9b), we seek the optimum L^*, defined as the one that minimizes the maximum error, $|s_p^* - s_p|_{\max}$, in a specified region of a thermodynamic diagram. At cold temperatures and hence small mixing ratios, $|s_p^* - s_p|$ is small because Y is small. We need to make this difference small at large r_s. For large mixing ratios, $|s_p^* - s_p|$ is small only if

$$L^*(T_K) + K_2 r_s(T_K, \theta_E) - L(T_K)$$
$$\approx \frac{c_w}{Y(T_K, \theta_E)} \int_{T_0}^{T_K} Y(\tau, \theta_E) \, d\tau, \quad (4.2)$$

where $L^* = L$ at the cold temperature T_0. For estimation of $L^* + K_2 r_s$, the quantity,

$$\Lambda \equiv L(T_K) + \frac{c_w}{Y(T_K, \theta_E)} \int_{T_0}^{T_K} Y(\tau, \theta_E) \, d\tau$$
$$= \frac{c_{pd}}{Y(T_K)} \ln \frac{\theta_E}{\theta_D} \quad (4.3)$$

[from (3.7)] was evaluated, using results from the numerical integration procedure described below. We may regard Λ as the data that $L^* + K_2 r_s$ should fit at large mixing ratios, and thus satisfy the approximation in (4.2).

The procedure (Bolton 1980) finds the true EPT of a parcel as follows. From (3.6), the differential equation defining a pseudoadiabat is

$$0 = d \ln \theta_E = d \ln \theta_x + \frac{c_w}{L(T_K)} \chi \, dT_K, \quad (4.4)$$

where $\ln \theta_x = \ln \theta_D + \chi$ and $\chi \equiv Lr_s/c_{pd}T_K$. The saturation vapor pressure is computed from (B10), the dewpoint temperature is calculated from the inverse of (B10), and the temperature at the LCL is given by (B15). The quantities θ_x and χ along a pseudoadiabat are found by numerically integrating (4.4) from the LCL where $\theta_x \equiv \theta_E'$, using the (second order) modified Euler method here and small temperatures steps. To reduce round-off error slightly, the prognostic variable in (B31) is changed here to $\ln(\theta_x/\theta_{x0})$ where θ_{x0} is the value of θ_x at $p = p_0$. At each step, χ is recovered from θ_x by solving (B32) via Newton's method. The pressure at each step is given by $p = e_s(1 + \varepsilon L/c_{pd}T_K\chi)$. The EPT of the pseudoadiabat is the value of θ_x obtained by integrating to a very cold temperature T_0 (in K) where the value of θ_x no longer changes.

5. Optimization procedure

First, consider formulas with two degrees of freedom, L_0^* and L_1^* ($K_2 = 0$). We seek the values of L_0^* and L_1^* that minimize the maximum absolute error $|\delta s|_{\max}$ in the region of a thermodynamic diagram defined by
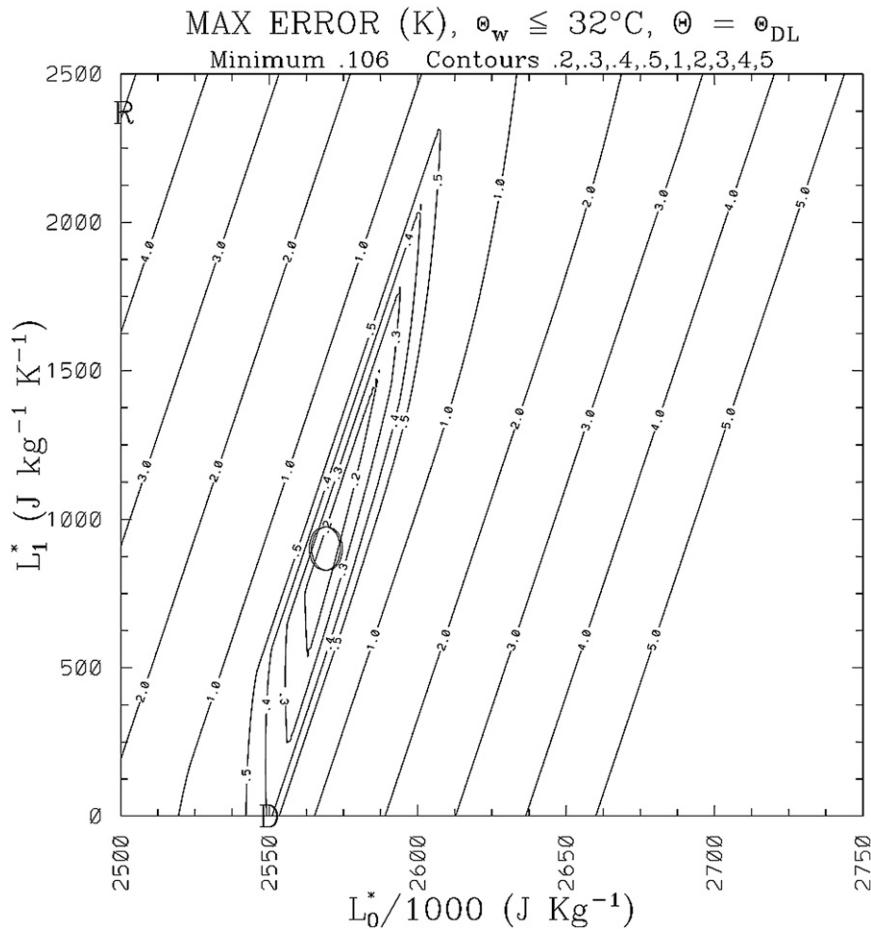
FIG. 1. Contours of $|\delta\theta_E|_{\max}$ in (L_0^*, L_1^*) space for $\Theta = \theta_{DL}$. The grid spacings are $\Delta L_0^* = 10^3$ J kg^{-1} and $\Delta L_1^* = 10$ J kg^{-1} K^{-1}. The contour levels and the minimum value in the 251 × 251 grid are shown at the top. The letters R, D, and the large O are centered on the points $(L_0, L_1) = (2501 \times 10^3, 2370)$ used in (2.4), $(L_0^*, L_1^*) = (2550.5 \times 10^3, 0)$ used in (6.2), and $(L_0^*, L_1^*) = (2569 \times 10^3, 900)$ used in (6.4), respectively (units are SI).

$100 \leq p \leq 1050$ mb and $\theta_w \leq 32°$C ($\theta_E \leq 400$ K). The procedure used to find the optimal values of the parameters L_0^* and L_1^* in a formula consists of the following steps.

1) Choose the set of grid points $\{-20°, -18°, \ldots, 32°C\} \times \{100, 125, \ldots, 1050$ mb$\}$ in (θ_w, p) space.
2) From the initial condition $T_K = \theta_w, p = p_0$, integrate along pseudoadiabats as described in section 3 to determine the true value of the EPT, θ_E, that corresponds to each WBPT, θ_w.
3) The integration procedure yields pressure on a regular grid in (θ_w, T_K) space. Obtain the values of temperature at the grid points in (θ_w, p) space by interpolation.
4) Select initial values for L_0^* and L_1^*.
5) Use the formula to compute the estimated EPT, θ_E^*, of a saturated parcel at each point.

6) At each point, calculate the difference $\delta\theta_E \equiv \theta_E^* - \theta_E$ between the EPT computed from the formula and the true EPT. Save $\delta\theta_E(\theta_w, p)$.
7) Find the maximum absolute difference $|\delta\theta_E|_{\max}$.
8) If the formula has two degrees of freedom, set up a mesh system in the 2D (L_0^*, L_1^*) space centered on the initial value with uniform spacing ΔL_0^* and ΔL_1^* directions. Repeat steps 4–7 at each grid point and contour the $|\delta\theta_E|_{\max}$ field. This is done for (2.7) with $K_2 = 0$ in Figs. 1 and 2 for a 251 × 251 grid in the domain defined by $L_0^* \in [2.5 \times 10^6, 2.75 \times 10^6]$ J kg^{-1} and $L_1^* \in [0, 2500]$ J kg^{-1} K^{-1}. At this high resolution it is evident that there is only one minimum in the domain when either $\Theta = \theta_{DL}$ (Fig. 1) or $\Theta = \theta$ (Fig. 2).
9) Record the minimum value and locate the grid point where it occurs. At this point center a new 251 × 251 grid with the spacing ΔL_0^* and ΔL_1^* reduced by

MAX ERROR (K), $\Theta_w \leqq 32°C$, $\Theta = \theta$
Minimum .18   Contours .3,.4,.5,1,2,3,4,5,10
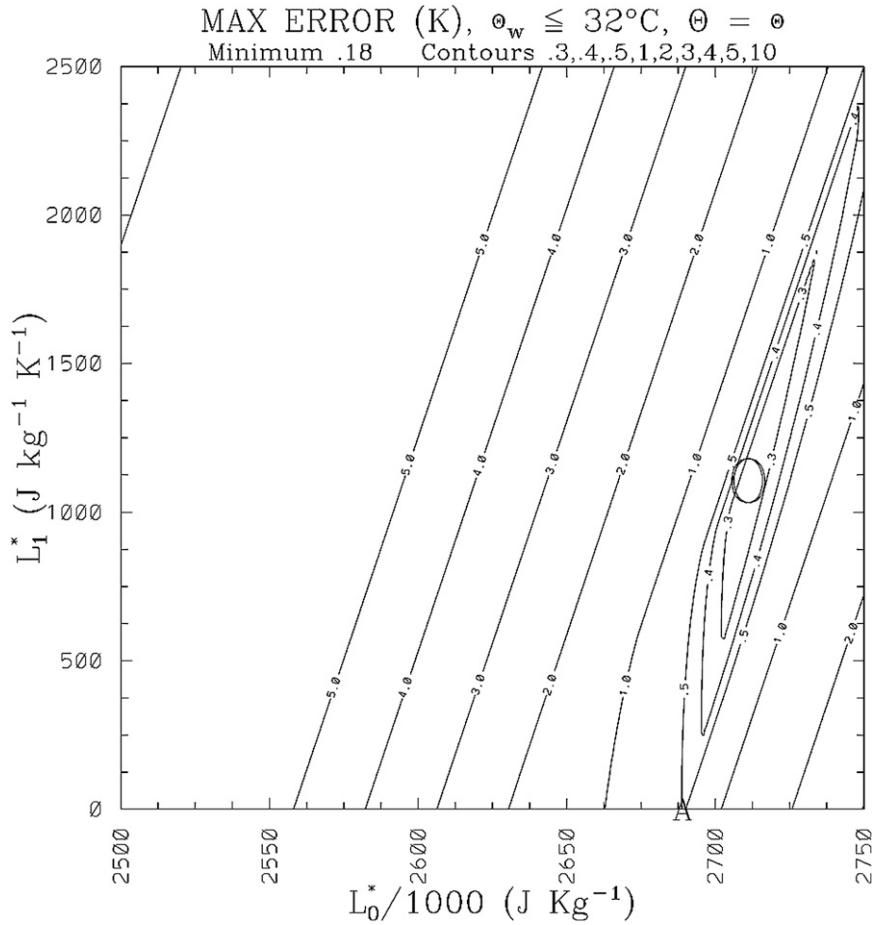
FIG. 2. As in Fig. 1, but for $\Theta = \theta$. The letters A and the large O locate the points $(L_0^*, L_1^*) = (2689.7 \times 10^3, 0)$ used in (6.1) and $(L_0^*, L_1^*) = (2711 \times 10^3, 1109)$ used in (6.3), respectively.

factors of 30 and 10, respectively, and find the minimum value and its location in this grid.

10) The optimum values of the parameters have now been determined. The accuracy E of the formula is the minimum value of $|\delta\theta_E|_{max}$ in (L_0^*, L_1^*) space. The parameters have to be found quite precisely because the error is sensitive to it [as found also by Bryan (2008)].

11) Data are also evaluated at points $\{\theta_w = 34°, 36°, 38°, 40°C\} \times \{p = 100, 125, \dots, 1050 \text{ mb}\}$ in a grid extension for plotting in some of the figures. These data are not used in optimization.

12) Steps 8–10 are similar for a formula with only one parameter L_0^*, except the search for the minimum is one dimensional (along the line $L_1^* = 0$). For the formula with three parameters, steps 8–10 are performed for different values of the third parameter, K_2, until the minimum in the 3D parameter space is found.

The method is quite general. It can be easily adapted to work with values of the physical constants and formulas for saturation vapor pressure and condensation temperature that differ from those that Bolton used.

6. Optimized formulas

We first consider the class of formulas with $L_1^* = 0$. The optimized version of (B35) is

$$\theta_E = \theta \exp\left(\frac{Ar}{T_L}\right), \quad A \equiv L_0^*/c_{pd} = 2674.5 \text{ K}, \quad (6.1)$$

where the optimum value of A is only slightly different from Bolton's value of 2675 K. Using θ_{DL} instead of θ provides us with a new more accurate formula:

$$\theta_E = \theta_{DL} \exp\left(\frac{L_0^* r}{c_{pd} T_L}\right), \quad (6.2)$$

TABLE 1. The formulas for θ_E and their errors. Here E is the maximum error in θ_E for saturated parcels in the region of a thermodynamic diagram defined by $-20°C \le \theta_w \le 32°C$ and $100\text{ mb} \le p \le 1050\text{ mb}$. The formulas are listed in order of increasing accuracy. The numbers in parentheses in the fourth column are the maximum errors for $\theta_w \le 40°C$.

Formula	Equation	Values of constants	E (K)	Degrees of freedom
(2.4)	$\theta_E = \theta_{DL} \exp\left[\dfrac{L_0 - L_1(T_L - C)}{c_{pd}T_L}r\right]$	$L_0 = 2.501 \times 10^6\text{ J kg}^{-1},$ $L_1 = 2370\text{ J kg}^{-1}\text{ K}^{-1}$	5.0 (11.1)	0
(Br13)	$\theta_E = \theta_D \mathcal{H}^{-\kappa_d r/\varepsilon} \exp\left(\dfrac{L_0^* r}{c_{pd}T}\right)$	$L_0^* = 2.555 \times 10^6\text{ J kg}^{-1}$	0.57 (0.73)	1
(6.1)	$\theta_E = \theta \exp\left(\dfrac{L_0^* r}{c_{pd}T_L}\right)$	$L_0^* = 2.6897 \times 10^6\text{ J kg}^{-1}$	0.49 (1.32)	1
(6.2)	$\theta_E = \theta_{DL} \exp\left(\dfrac{L_0^* r}{c_{pd}T_L}\right)$	$L_0^* = 2.5505 \times 10^6\text{ J kg}^{-1}$	0.38 (0.84)	1
(6.3)	$\theta_E = \theta \exp\left[\dfrac{L_0^* - L_1^*(T_L - C)}{c_{pd}T_L}r\right]$	$L_0^* = 2.711 \times 10^6\text{ J kg}^{-1},$ $L_1^* = 1109\text{ J kg}^{-1}\text{ K}^{-1}$	0.18 (1.66)	2
(6.4)	$\theta_E = \theta_{DL} \exp\left[\dfrac{L_0^* - L_1^*(T_L - C)}{c_{pd}T_L}r\right]$	$L_0^* = 2.569 \times 10^6\text{ J kg}^{-1},$ $L_1^* = 900\text{ J kg}^{-1}\text{ K}^{-1}$	0.11 (1.28)	2
(B38)**	$\theta_E = \theta \exp\left[\dfrac{L^* r}{c_{pd}T_L}(1 + k_2 r)\right]$	$L_0^* = 2.6975 \times 10^6\text{ J kg}^{-1},$ $L_1^* = 2554.5\text{ J kg}^{-1}\text{ K}^{-1},$ $k_2 = 0.810$	0.085 (0.94)	2
(B39)	$\theta_E = \theta_{DL} \exp\left[\dfrac{L^* r}{c_{pd}T_L}(1 + k_2 r)\right]$	$L_0^* = 2.5643 \times 10^6\text{ J kg}^{-1},$ $L_1^* = 1790\text{ J kg}^{-1}\text{ K}^{-1},$ $k_2 = 0.448$	0.036 (0.104)	3
(6.5)	$\theta_E = \theta_{DL} \exp\left[\dfrac{(L^* + K_2 r)r}{c_{pd}T_L}\right]$	$L_0^* = 2.56313 \times 10^6\text{ J kg}^{-1},$ $L_1^* = 1754\text{ J kg}^{-1}\text{ K}^{-1},$ $K_2 = 1.137 \times 10^6\text{ J kg}^{-1}$	0.015 (0.095)	3

** (B38) has only two degrees of freedom because $L^* = 1.0784L$.

where $L_0^* = 2.5505 \times 10^6\text{ J kg}^{-1}$ is the optimum value, which is close to the value $2.555 \times 10^6\text{ J kg}^{-1}$ obtained by Bryan (2008) despite the different optimization criteria.

Optimizing (2.7) with $K_2 = 0$ and two degrees of freedom, L_0^* and L_1^*, results in the new formulas:

$$\theta_E = \theta \exp\left[\frac{L_0^* - L_1^*(T_L - C)}{c_{pd}T_L}r\right],$$

$$\begin{cases} L_0^* = 2.711 \times 10^6\text{ J kg}^{-1} \\ L_1^* = 1109\text{ J kg}^{-1}\text{ K}^{-1} \end{cases} \quad (6.3)$$

and

$$\theta_E = \theta_{DL} \exp\left[\frac{L_0^* - L_1^*(T_L - C)}{c_{pd}T_L}r\right],$$

$$\begin{cases} L_0^* = 2.569 \times 10^6\text{ J kg}^{-1} \\ L_1^* = 900\text{ J kg}^{-1}\text{ K}^{-1} \end{cases}. \quad (6.4)$$

In addition, a new formula with three degrees of freedom is found:

$$\theta_E = \theta_{DL} \exp\left\{\frac{[L_0^* - L_1^*(T_L - C) + K_2 r]r}{c_{pd}T_L}\right\}, \quad (6.5)$$

where $L_0^* = 2.56313 \times 10^6\text{ J kg}^{-1}$, $L_1^* = 1754\text{ J kg}^{-1}\text{ K}^{-1}$, and $K_2 = 1.137 \times 10^6\text{ J kg}^{-1}$.

7. Accuracy of the formulas

The previous and new formulas are ranked in terms of the accuracy E in Table 1 and their maximum errors as functions of θ_w are shown in Figs. 3–5. The accuracies of the formulas in the region $100 \le p \le 1050\text{ mb}$ and $\theta_w \le 32°C$ are determined first of all by the number of degrees of freedom and then, with one exception, by the choice for Θ as anticipated in section 3. The Rossby equation (2.4), which has no degrees of freedom, shows the maximum error (up to 5 K in the above region) that
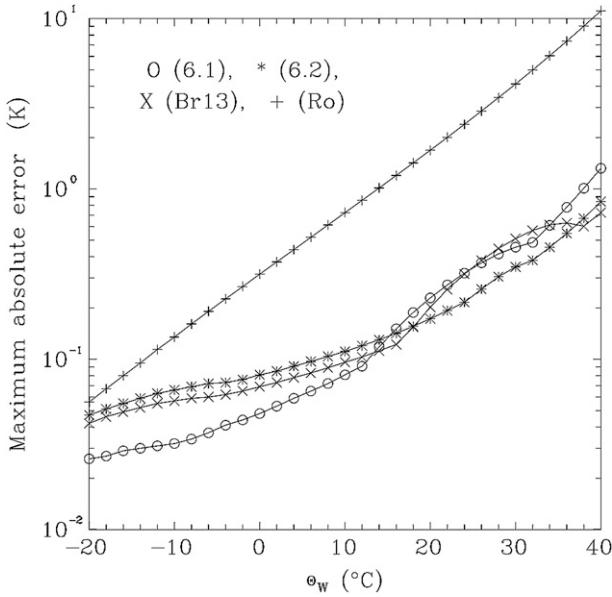
FIG. 3. Maximum absolute error $|\theta_E^* - \theta_E|$ as a function of θ_w for the Rossby formula, (Ro) or (2.4), which has no degrees of freedom, and for the Eqs. (6.1), (6.2), and (Br13) that have one degree of freedom. The ordinate scale is logarithmic.

FIG. 4. As in Fig. 3, but for (B38), (6.3), and (6.4), which have two degrees of freedom.

arises from neglecting the c_w term and utilizing the actual latent heat. The Rossby formula has a maximum error with respect to pressure (with θ_w held fixed) that varies almost exponentially with θ_w (Fig. 3).

Of the formulas with a constant adjusted latent heat (one degree of freedom), (6.2) has the least maximum error, 0.38 K (Fig. 3) because it uses θ_{DL}. The modified Betts–Dugan equation (6.1), which contains θ, is accurate to 0.49 K. Even though it has the same form as (6.2) for a saturated parcel, Bryan's formula (Br13) with a maximum error of 0.57 K is slightly less accurate than (6.1). This is probably due to it being optimized by minimizing the mean square error (instead of the maximum error) for a limited number of cases.

Because it uses θ, (6.3) with a maximum error of 0.18 K is the least accurate of the formulas with two degrees of freedom (Fig. 4). Even though it also uses θ and (6.4) uses θ_{DL}, (B38) is slightly the more accurate with a maximum error of 0.09 K compared to 0.11 K. The better accuracy of (B38) is probably because of its use of k_2 [see (2.1)] as the second adjustable parameter and because of the fixed parameter L_1^* being determined by $L^* \propto L$ instead of being set to zero.

In the category with three degrees of freedom, (6.5) is accurate to 0.15 K and (B39) to 0.035 K (Fig. 5). However, (B39) is more accurate for $\theta_w < 24°$C so there is little to choose between the two formulas. Surprisingly, (B38) is used most frequently (Emanuel 1994; Bryan 2008) even though it is less accurate than (B39).

The maximum errors are not restrained by optimization beyond $\theta_w = 32°$C and grow rapidly (Figs. 3–5). For $\theta_w \leq 40°$C, the widely used Eq. (B38) has a maximum error of 0.94 K (Table 1). In contrast, (6.5) and (B39) contain the error to 0.1 K (Fig. 5).

The quantity Λ defined by (4.3) is the "adjusted latent heat according to the data." Figure 6 is a scattergram of
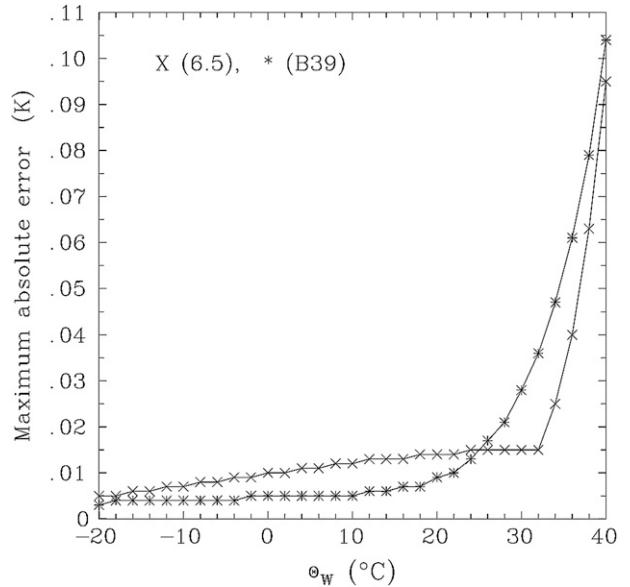
FIG. 5. As in Fig. 3, but for (6.5) and (B39), which have three degrees of freedom, and the ordinate scale is now linear.
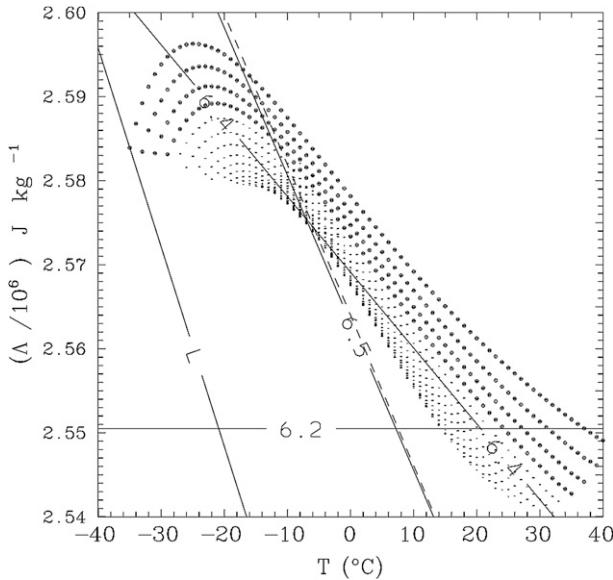
FIG. 6. Scatter diagram for $\Lambda \equiv c_{pd} \ln(\theta_E/\theta_D)/Y$ vs temperature T (°C) for data at all the points in the grid for which $r_s \geq 0.002$ (small dots) and at the points in the grid extension (circled dots). The lines identified by L, (6.2), (6.4), and (6.5) and the dashed line [near the (6.5) line] are the actual latent heat of vaporization according to (B2), the constant adjusted latent heat used in (6.2), and the adjusted latent heats used in (6.4), (6.5), and (B39), respectively. The data for $\theta_w > 32$°C is not used in the determination of the adjusted latent heats (and K_2).

Λ versus T for all the points in the grid for which $r_s \geq 0.002$. Lower values of r_s were excluded because $\Lambda \to 0/0$ as $r_s \to 0$. The data do not lie precisely on a straight line, indicating that, although Λ is mainly a linear function of T_K, it is slightly dependent on r. The straight lines are the actual latent heat, $L = L_0 - L_1 T$ used in (2.4), the constant latent heat, $L^* = L_0^*$, used in (6.2), and the adjusted latent heats, $L^* = L_0^* - L_1^* T$, used in (6.4), (6.5), and (B39). The constant latent heat used in (6.2) is equal to the computed adjusted latent heats within a few degrees of 20°C. The line for (6.4) fits the data well. The (6.5) and (B39) lines are not a good fit at cold temperatures (and small mixing ratios), but this is not crucial because L^* is multiplied by r in the formulas. These lines underestimate the observed adjusted latent heats at warm temperatures to make room for functions of r, which are not represented in Fig. 6. Figure 7 is a scattergram for Λ/L^*(B39) versus r_s to isolate the $(1 + k_2 r)$ factor in (B39) according to the data. The points spread out at small mixing ratio as the numerator and denominator both tend to zero. Bolton's line $1 + 0.448 r_s$ fits the data nicely, thus verifying (B39). Similarly a scattergram for $\Lambda - L^*$(6.5) versus r_s (Fig. 8) isolates the $K_2 r$ term in (6.5) according to the data. The line $K_2 r_s$, $K_2 = 1.137 \times 10^6$ J kg^{-1}, obtained by optimization, is also a good fit to the data.
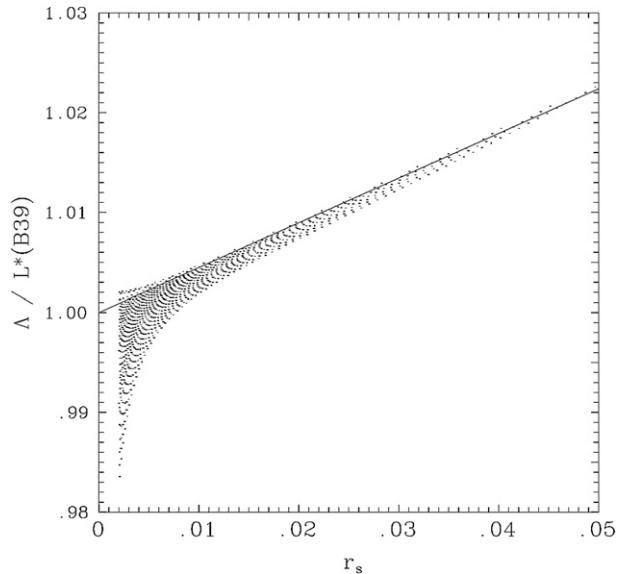
FIG. 7. Scatter diagram for Λ/L^*(B39) vs r_s for the same data points as in Fig. 6, where L^*(B39) is the adjusted latent heat in (B39). Also shown is the line Λ/L^*(B39) = $1 + k_2 r_s$, $k_2 = 0.448$, which is Bolton's fit to the data.

For formulas with $L_1^* = k_2 = K_2 = 0$, it is apparent from (2.7) that the adjusted latent heat for a formula that uses θ must be larger than the corresponding formula that uses θ_{DL} by an amount that is approximately equal to $(c_{pd} T_L/r) \ln(\theta_{DL}/\theta)$. Over the grid this quantity ranges from 1.2×10^5 to 1.6×10^5 J kg^{-1} with a mean around
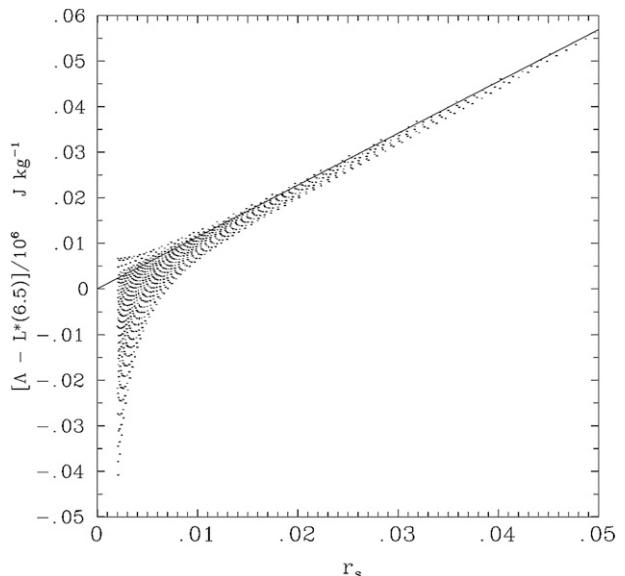
FIG. 8. Scatter diagram for $\Lambda - L^*$(6.5) vs r_s for the same data points as in Fig. 6, where L^*(6.5) is the adjusted latent heat in (6.5). Also shown is the line $[\Lambda - L^*(6.5)] = K_2 r_s$, $K_2 = 1.137 \times 10^6$ J kg^{-1}, used in (6.5).

1.4×10^5 J kg^{-1}. From Table 1 we see that this agrees with the difference (1.39×10^5 J kg^{-1}) between L_0^* for (6.1) and (6.2).

Finally, we stress that all the accuracies given above are relative to the results from numerical integration of (B25). Owing to c_{pd} not being strictly constant, there is an uncertainty of up to 0.2 K, which has not been taken into account (Bolton 1980).

8. Summary

The accuracies of several formulas for equivalent potential temperature have been assessed by computing their maximum error throughout the region of a thermodynamic diagram defined by $100 \leq p \leq 1050$ mb and $\theta_w \leq$ 32°C ($\theta_E \leq 400$ K). The more accurate formulas contain θ_{DL} rather than θ, and T_L, not $\mathcal{H}$. Some new formulas have been devised. These have two or three degrees of freedom and minimize the above maximum error. With one degree of freedom, a constant latent heat, it is possible to fit the data to 0.4 K. This error is reduced to 0.1 K [in (6.4)] by utilizing an adjusted latent heat that depends linearly with temperature. The residual error is not a function of temperature. It must therefore be a function of r since T_L and r alone (or T_K and r_s if the parcel is saturated) determine θ_E. To achieve greater accuracy than 0.1 K, a formula must contain this extra dependence on r. Bolton's (B38) and (B39) do so by containing an r^2 term. Equation (B39) is the more accurate because it uses θ_{DL} and has an extra degree of freedom.

Finding the imitation first law of thermodynamics that the formulas satisfy approximately reveals how the formulas work. Adjusting the adjusted specific heat of water to zero to eliminate the integral term in the entropy formulation and Kirchoff's equation makes the specific heat of water vapor negative (or zero if the formula uses a constant latent heat). Thus, the specific heat of moist air is reduced artificially. An artificial increase in latent heat, $(L^* - L)\,dr$, is required to compensate for the decrease in specific heat.

The highly accurate Eqs. (B38) and (B39) are not easily reconciled with an imitation first law. Therefore, a formula, (6.5), is devised herein that has a slightly simpler formula than (B39), has comparable accuracy, and can be related to an imitation first law if a small r^2 term is added to the imitation enthalpy. This small boost in enthalpy is additional compensation that is needed at high mixing ratios.

APPENDIX

List of Symbols

A = 2675 K, the constant in (B35).

C = 273.15 K (absolute zero = 0 K = −273.15°C).

E: Maximum absolute error in θ_E for $\theta_w \leq 32$°C, $100 \leq p \leq 1050$ mb.

$\mathcal{H}$: Relative humidity $\equiv e/e_s$.

K_2: A constant in (2.7) and (6.5) = 1.137×10^6 J kg^{-1} in (6.5).

$L(T_K)$: Latent heat of vaporization, $= L_0 - L_1(T_K - C)$.

$L_0 = 2.501 \times 10^6$ J kg^{-1}.

$L_1 = 2370$ J kg^{-1} K^{-1} ($\approx c_w - c_{pv}$, Kirchoff's equation).

L^* Adjusted latent heat, $= L_0^* - L_1^*(T_K - C)$.

Q: Total water mixing ratio (g g^{-1}).

R_d: Gas constant for dry air = 287.04 J kg^{-1} K^{-1}.

R_m: Gas constant for moist air = $R_d(1 + r/\varepsilon)/(1 + r) \approx R_d(1 + 0.608r)$.

R_v: Gas constant for water vapor = 461.50 J kg^{-1} K^{-1} ($= R_d/\varepsilon$).

T, T_K: Temperature (°C and K, respectively).

T_L: Temperature at the LCL (K).

T_0: A very cold temperature (K).

$Y \equiv r/T_K$ (K^{-1}).

c_{pd}: Specific heat at constant pressure of dry air = 1005.7 J kg^{-1} K^{-1} ($= 3.504\,R_d$).

c_{pm}: Specific heat at constant pressure of moist air = $(c_{pd} + rc_{pv})/(1 + r) = c_{pd}(1 + 0.887r)$.

c_{pv}: Specific heat at constant pressure of water vapor = 1875 J kg^{-1} K^{-1} ($\approx 4R_v$).

c_{pv}^*: Adjusted value of $c_{pv} = -L_1^*$.

c_w, c_w^*: Specific heat of water, = 4190 J kg^{-1} K^{-1} and adjusted value (= 0).

e: Vapor pressure (mb), $e = e_s(T_D)$, T_D = dewpoint temperature (K).

$e_s(T_K)$: Saturation vapor pressure (mb) = $6.112 \times \exp[17.67(T_K - C)/(T_K - C + 243.5)]$.

$de_s/dT_K = Le_s/R_v T_K^2$ (Clausius–Clapeyron equation).

h, h^*: Specific enthalpy, adjusted specific enthalpy (J kg^{-1}).

k_2: A nondimensional constant equal to 0.81 in (B38) and 0.448 in (B39).

p: Pressure (mb).

p_0: = 1000 mb.

r: Mixing ratio (g g^{-1}), $= \varepsilon e/(p - e)$.

r_s: Saturation mixing ratio (g g^{-1}) = $\varepsilon e_s/(p - e_s)$.

r_w: Liquid water mixing ratio (g g^{-1}).

s_p, s_p^*: Actual and adjusted specific pseudoadiabatic entropy.

s_r: Total (reversible) specific entropy of moist air $\equiv s_d + rs_v + r_w s_w$.

$\Delta L_0^*, \Delta L_1^*$: Grid spacings in ($L_0^*, L_1^*$) space.

Λ: Defined in (4.3).

Θ: Either θ or θ_{DL}.

α_d: Specific volume of dry air (m^3).

$\chi \equiv L r_s / c_{pd} T_K$.

$\varepsilon = R_d / R_v = 0.6220$.

$\kappa_d = R_d / c_{pd} = 0.2854 \; (\approx 2/7)$.

$\kappa_m = R_m / c_{pm} = \kappa_d (1 - 0.28r)$.

θ: Potential temperature of moist air (K) $= T_K (p_0/p)^{\kappa_m}$.

θ_D: Potential temperature of dry air (K) $= T_K [p_0/(p - e)]^{\kappa_d}$.

θ_{DL}: Value of θ_D at the LCL (K).

θ_E, θ_E': EPT and Rossby EPT (K).

θ_E^*: Estimate of θ_E by a formula.

θ_w: Wet-bulb potential temperature (WBPT) (°C).

$\theta_x \equiv \theta_D \exp(\chi)$.

$|\delta \theta_E|_{max}$: Maximum error in θ_E as a function of L_0^* and L_1^*.

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