

On the Computation of Pseudoadiabatic Entropy and Equivalent Potential Temperature

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ABSTRACT

A set of approximate equations for pseudoadiabatic thermodynamics is developed. The equations are derived by neglecting the entropy of water vapor and then compensating for this error by using a constant (but relatively large) value for the latent heat of vaporization. The subsequent formulations for entropy and equivalent potential temperature have errors that are comparable to those of previous formulations, but their simple form makes them attractive for use in theoretical studies. It is also shown that, if the latent heat of vaporization is replaced with a constant value, an optimal value should be chosen to minimize error; a value of $2.555 \times 10^6 \text{ J kg}^{-1}$ is found in tests herein.

1. Introduction

It is possible to derive several different thermodynamical variables that are conserved during moist adiabatic processes. The most commonly used variable in research and operational forecasting is equivalent potential temperature, or θ_e . Conceptually, θ_e is the potential temperature an air parcel would have if all the water vapor were condensed by lifting the parcel to zero pressure. (Typically, the ice phase is neglected, and any freezing of the condensed water at low temperatures is not considered; this assumption is also made herein.)

There are numerous mathematical formulations for θ_e in the atmospheric sciences literature. Most of them are approximate formulations of varying degrees of accuracy. In the next section, a review is provided of the two most accurate formulations, which are applicable to very different physical situations. One, originally developed by Iribarne and Godson (1973), is appropriate for nonprecipitating clouds. It has the nice property of being an exact formulation (under the physical processes considered). A second formulation, presented by

Bolton (1980), is appropriate for clouds that are precipitating. However, it is an empirical formulation based on fits to numerically generated data; consequently, this formulation has been difficult to apply in certain theoretical studies.

The primary purpose of this article is to demonstrate that a reasonably accurate formulation for θ_e that is applicable to precipitating clouds can be derived with a small number of reasonable assumptions. The subsequent formulation has accuracy that is comparable to other approximate formulations, but has the distinct advantage of having consistent formulations for other thermodynamical variables (e.g., total moist entropy and enthalpy). The new formulation is reasonably accurate, inexpensive, adaptable, and attractive for theoretical studies, which is a combination of characteristics that may be unrivaled by all other formulations that have been presented previously.

2. Review

Before developing a mathematical formula for θ_e , several assumptions must be made about what processes are considered during condensation. For simplicity, the ice phase is typically neglected, and this assumption is also made herein. Another common assumption is that all phases of water shall be in equilibrium during condensation. Consequently, supersaturation is not permitted. Third, a critical assumption must be made about the fate of condensed water. This is a complex

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problem because liquid water can fall relative to air. Two cases represent the extreme ends of the spectrum: 1) all condensate moves with the air (and, thus, there is no precipitation), or 2) all condensate immediately falls relative to the air (and, thus, precipitation is instantaneous). These processes are considered separately in sections 2a and 2b.

a. Reversible thermodynamics

On one extreme, if all liquid water moves with the parcel, then this water could then be available later for evaporation. Hence, a parcel of cloudy air could be brought back to its original state via evaporation. This is a *reversible moist adiabatic* process. It is probably most applicable to shallow clouds and cumulus congestus in which precipitation is negligible. The mathematics of reversible moist adiabatic processes are tractable, and can be found in several texts (e.g., Iribarne and Godson 1981; Emanuel 1994). In this case, the mathematical formulation of total moist entropy (hereinafter referred to as reversible moist entropy, or s^r) is given by

$$s^r = (c_p + c_l r_l) \ln T - R \ln p_d + \frac{L_v r_v}{T} - R_v r_v \ln(\mathcal{H}), \quad (1)$$

where the symbols are defined as follows: T is absolute temperature; p_d is the partial pressure of dry air; R and R_v are respectively the gas constants for dry air and water vapor; c_p is the specific heat at constant pressure for dry air; c_l is the specific heat of liquid water; r_v and r_l are respectively the mixing ratios of water vapor and total water; $\mathcal{H} \equiv e/e_s$ is relative humidity, where e is the partial pressure of water vapor and e_s is the value of e at saturated equilibrium at the same temperature; and L_v is the latent heat of vaporization, which is a function of temperature according to Kirchoff's Law: $dL_v/dT = c_{pv} - c_l$, where c_{pv} is the specific heat of water vapor at constant pressure.

Equivalent potential temperature θ_e is simply a different measure of entropy. Hereinafter, θ_e during reversible adiabatic conditions is referred to as *reversible equivalent potential temperature*, or θ_e^r . The variables s^r and θ_e^r are related as

$$(c_p + c_l r_l) \ln \theta_e^r \equiv s^r + R \ln p_0, \quad (2)$$

where p_0 is a reference pressure (typically 1000 hPa). From (1) and (2), it follows that θ_e^r has an exact mathematical formulation:

$$\theta_e^r = T \left(\frac{p_0}{p_d} \right)^{R/(c_p + c_l r_l)} \mathcal{H}^{-R_v r_v / (c_p + c_l r_l)} \exp \left[\frac{L_v r_v}{(c_p + c_l r_l) T} \right]. \quad (3)$$

Under strictly saturated conditions (i.e., $\mathcal{H} = 1$), the mathematical formulation for s^r was first presented by Iribarne and Godson (1973), and (3) with $\mathcal{H} = 1$ was first presented by Paluch (1979). In Paluch's article, and in many other places, θ_e^r is referred to as "wet equivalent potential temperature." The terms with \mathcal{H} in (1) and (3) were added by Emanuel (1994) to account for conservation in subsaturated conditions.

b. Pseudoadiabatic thermodynamics

On the other extreme, it can be assumed that all condensed water is immediately removed from a parcel. This is an irreversible process because, consequently, there is no water available for evaporation; thus, a warming (i.e., descending) parcel of air would follow dry adiabatic processes, not a saturated process, and thus a parcel could not be brought back to its original conditions. Following convention, this is referred to as a *pseudoadiabatic process*. Entropy and θ_e during this process are hereinafter referred to as pseudoadiabatic moist entropy s^p and pseudoadiabatic equivalent potential temperature θ_e^p . Because deep cumulus convection typically produces precipitation, these variables are probably most applicable to deep (of order 10 km) clouds. However, they will never be strictly conserved in such clouds because *some* liquid water is inevitably lofted by convective updrafts.

The mathematical formulations for s^p and θ_e^p are more complicated than their counterparts from reversible thermodynamics because total water is not constant along a pseudoadiabatic. Most derivations of s^p begin by taking the differential of (1) and then neglect the term involving liquid water mixing ratio r_l (because liquid water is immediately removed from air by fallout); this yields

$$ds^p = (c_p + c_l r_v) d \ln T - R d \ln p_d + d \left(\frac{L_v r_v}{T} \right) - R_v d[r_v \ln(\mathcal{H})]. \quad (4)$$

Integration of this equation results in a formulation for s^p :

$$s^p = c_p \ln T + c_l \int_{T_0}^T r_v d \ln(T) - R \ln p_d + \frac{L_v r_v}{T} - R_v r_v \ln(\mathcal{H}) \quad (5)$$

(see also Iribarne and Godson 1981, p. 143) wherein integration is performed around a reference state at a very small temperature T_0 , such that the constants of integration are essentially zero. The term with the integral in (5) makes s^p expensive to calculate. Further-

more, any attempts to create a mathematical definition of θ_e^p from (5) would result in a similarly complex and expensive variable. Consequently, terms are usually omitted from these formulations, or approximations to certain terms are made, to circumvent the need for expensive calculations; however, these approximations introduce errors of various degrees. Hence, there are

many different approximate mathematical formulations for θ_e^p in the literature (e.g., Betts and Dugan 1973; Simpson 1978; Bolton 1980).

Using a numerical code, Bolton (1980) used (4) to produce a dataset of pseudoadiabatic conditions. He then fit empirical functions to the results, and derived the approximate formulation

$$\theta_e^p \approx T \left(\frac{p_0}{p} \right)^{0.2854(1-0.28r_v)} \exp \left[\left(\frac{3376}{T_L} - 2.54 \right) r_v (1 + 0.81r_v) \right], \tag{6}$$

where T_L is absolute temperature at the lifting condensation level. Bolton (1980) determined that (6) is accurate to within 0.3 K. Because of its superior accuracy relative to other approximate formulations, this has become a very popular mathematical formulation for θ_e^p .

A consistent formulation for s^p was not presented by Bolton (1980). However, by analogy to the derivation in reversible conditions, a formulation for s^p can be obtained by working backward from (6); that is

$$s^p \approx c_p \ln \theta_e^p - R \ln p_0. \tag{7}$$

Using a numerical code (explained in a later section), the author has found that both θ_e^p and s^p , as defined by (6) and (7), are conserved well in pseudoadiabatic conditions.

There are two practical problems with using these formulations, however. First, Bolton (1980) derived (6) using certain formulations for $e_s(T)$ and other mathematical constants (R , c_p , etc.). Thus, (6) is not directly applicable to situations that use different formulations (for e_s , R , c_p , etc.). For example, if (6) is used with output from a numerical cloud model that uses different formulations, then some error may be incurred.

The second problem is that these formulas are inconvenient for analytic studies that require moist thermodynamical expressions. As an example, Emanuel (1994, p. 124) used the mathematical formulation for entropy to derive a set of Maxwell relations. These equations can then be used in numerous ways, such as for the derivation of the moist adiabatic lapse rate. These Maxwell relations are also crucial for certain theoretical work, such as the analytical theory for the maximum possible intensity of tropical cyclones (Emanuel 1986, 1988). The complex form of (6) and (7) makes them impractical to use for such studies.

In summary, (6) and (7) may be very accurate and sufficient for most applications. However, their empirical derivation means they are not flexible (e.g., for use

with different underlying thermodynamic formulations) and they are not tractable for analytical studies.

3. An approximation for pseudoadiabatic thermodynamics

Based on the preceding review, there appears to be a need for formulations of s^p and θ_e^p that are accurate, adaptable, and yet relatively simple so that they can be used for theoretical studies. To this end, a new derivation begins with a formula that governs entropy changes in pseudoadiabatic conditions (Emanuel 1994, p. 131):

$$T ds^p = (c_p + c_{pv} r_v) dT + L_v dr_v - \alpha_d dp, \tag{8}$$

where α_d is the specific volume of dry air. This equation is derivable from (4) by using Kirchoff's equation and the Clausius–Clapeyron equation. It is assumed that s^p is constant under any processes considered herein (and thus $ds^p = 0$). For simplicity, the simple case of condensation with pressure held constant ($dp = 0$) is considered first. (In other words, the saturated enthalpy is considered first.) Additionally, the latent heat of vaporization is written relative to a constant value L_0 , for reasons that will become clear later; that is, $L_v(T) \equiv L_0 + L^*(T)$. Under these assumptions, and after rearranging some terms, (8) can be expressed as

$$c_p \underbrace{\left(1 + \frac{c_{pv}}{c_p} r_v \right)}_{\epsilon_1} dT = -L_0 \underbrace{\left(1 + \frac{L^*}{L_0} \right)}_{\epsilon_2} dr_v. \tag{9}$$

Assuming L_0 is $O(2.5 \times 10^6 \text{ J kg}^{-1})$, then under all atmospheric conditions both terms in parentheses (ϵ_1 and ϵ_2) are of order 1. Thus, it would be reasonably accurate to set $\epsilon_1 = \epsilon_2 = 1$ to simplify calculations (e.g., Iribarne and Godson 1981, p. 142). In fact, making this assumption eliminates the expensive integral term in (5), which represents the contribution to entropy from

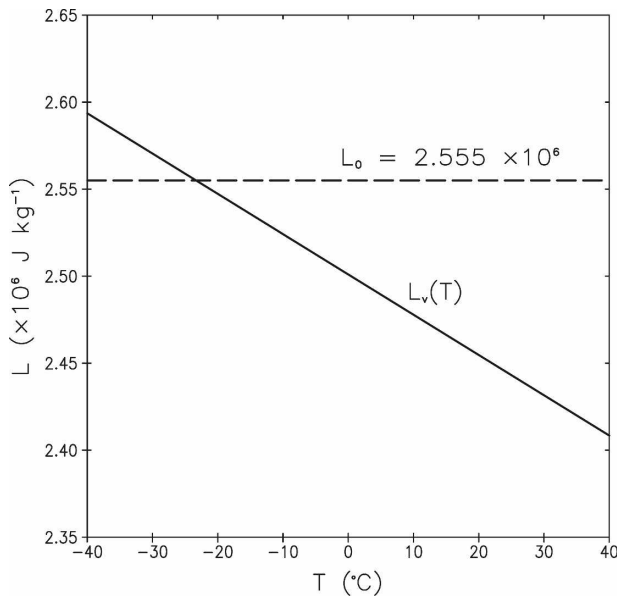


FIG. 1. Latent heat of vaporization: $L_v(T)$ (solid) and L_0 (dashed).

water vapor. On the other hand, some error is incurred by making this assumption, although the error may be minimal for some applications. However, in deep moist convection total condensation is relatively large, and the error incurred by making such assumptions can become unacceptable [as shown, e.g., by Wilhelmson (1977) and Tripoli and Cotton (1981)].

Serendipitously, the value of L_0 is unconstrained; that is, it can be set to *any* value (provided that L^* is redefined appropriately). Furthermore, changes in L_0 imply changes in ϵ_2 . It is possible, then, to choose a value for L_0 such that $\epsilon_2 \approx \epsilon_1$ across a broad range of environments. In other words, the error incurred by one assumption (i.e., neglecting the contribution to entropy by water vapor) can be compensated by another assumption (i.e., neglecting the temperature dependence of L_v). Thus, the primary approximation changes from $\epsilon_1 = \epsilon_2 = 1$ to $\epsilon_1 \approx \epsilon_2$. Although several previous studies have used a constant value for L_v (analogous to the value L_0 herein), it may be a novel idea to adjust L_0 to compensate errors in approximate thermodynamic expressions.

To aid in the following discussion, Fig. 1 displays the variation in L_v as a function of temperature (solid line). If L_0 is chosen as a relatively large value (as shown in Fig. 1), then ϵ_2 would be small at low temperatures; this situation is convenient, because ϵ_1 is small at low temperatures (because r_v is typically small). Thus, $\epsilon_1 \approx \epsilon_2$, and both terms drop out of (9).

At relatively high temperatures, r_v can be $O(0.02)$ and thus $\epsilon_1 \approx 1.05$. In the case shown in Fig. 1, at high

temperatures $\epsilon_2 \approx 0.95$. So, at this temperature, these two variables are still of order 1, but the agreement is not quite as good. Nevertheless, it is still the case that $\epsilon_1 \approx \epsilon_2$, and thus both terms can be assumed to drop out of (9) with reasonable accuracy.

It follows, then, that the approximate equation,

$$Tds^p \approx c_p dT + L_0 dr_v - \alpha_d dp, \quad (10)$$

should provide accurate results for pseudoadiabatic processes, provided that L_0 is adjusted to an optimal value to ensure minimal errors. This optimal value for L_0 is determined numerically later in this article.

Dividing (10) by T , using the Clausius–Clapeyron equation, Kirchoff’s equation, and the equation of state, and finally integrating from very low temperatures, an approximate formulation for s^p is obtained:

$$s^p \approx c_p \ln T - R \ln p_d + \frac{L_0 r_v}{T} - R_v r_v \ln(\mathcal{H}). \quad (11)$$

This formulation for s^p is very similar to the formulation for s^r [given by (1)], except the term with c_l is omitted and L_v is replaced by L_0 . In this case, the relationship between s and θ_e is given as

$$c_p \ln \theta_e^p \equiv s^p + R \ln p_0. \quad (12)$$

Consequently, the mathematical formulation for θ_e is

$$\theta_e^p \approx T \left(\frac{p_0}{p_d} \right)^{R/c_p} \mathcal{H}^{-R_v r_v / c_p} \exp \left(\frac{L_0 r_v}{c_p T} \right). \quad (13)$$

As with s^p , this formulation for θ_e^p is very similar to its reversible counterpart [given by (3)], except that all terms with c_l are omitted and L_v is replaced by L_0 .

It is interesting to note that the same approximations are made in many numerical cloud models. That is, in many cloud models the terms involving c_l are omitted from the thermodynamic equation, and $L_v(T)$ is replaced with a constant value (although, the first of these two approximations is more common). The analysis herein suggests that these are adequate assumptions for heavily precipitating cases (i.e., cases wherein the pseudoadiabatic assumption is appropriate). The analysis herein further suggests that an optimal value for L_0 can be chosen, such that $\epsilon_1 \approx \epsilon_2$ for a broad range of atmospheric conditions. This optimal value is determined during numerical tests in a later section of this article.

4. Numerical evaluation

To evaluate the accuracy of the approximate equations derived in the previous section, a numerical code

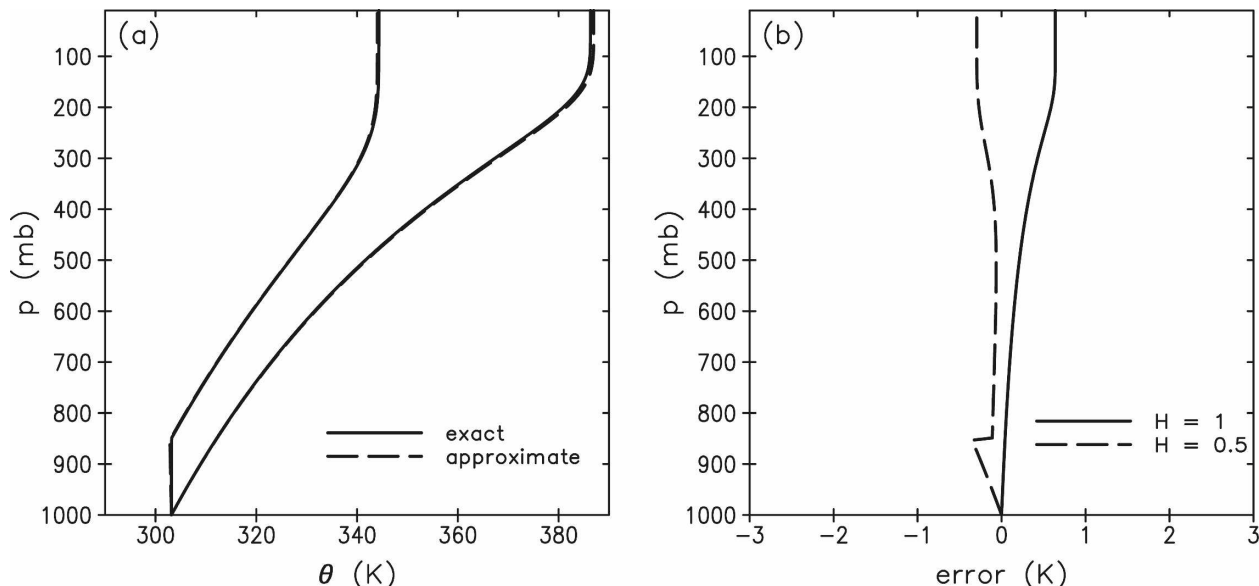


FIG. 2. Output from the numerical code. (a) Potential temperature along a pseudoadiabat using the exact formulation (solid) and using the approximate formulation (dashed). All cases begin at $p = 1000$ hPa and $T = 30^\circ\text{C}$, but the curves on the right begin with $\mathcal{H} = 1$ and the curves on the left begin with $\mathcal{H} = 0.5$. (b) Potential temperature errors using the approximate equation, where the solid line is the case beginning with $\mathcal{H} = 1$ and the dashed line is the case beginning with $\mathcal{H} = 0.5$.

is used to generate moist adiabats under various conditions. The code was described in detail by Bryan and Fritsch (2004). They used it to evaluate several formulations of ice–liquid water potential temperature, but it is easily adapted to evaluate θ_e .

The fundamental equation for this code can be expressed as follows:

$$(c_p + c_{pv}r_v + c_r r_l)d \ln T = (R_d + R_v r_v)d \ln p - \frac{L_v}{T} dr_v. \tag{14}$$

This equation governs reversible processes, but it can be used for pseudoadiabatic conditions if liquid water is immediately removed upon formation [as was done by Bolton (1980)]. The only modifications to the code from what was reported by Bryan and Fritsch (2004) are the values used for gas constants and specific heats, and the formulations for $L_v(T)$ and $e_s(T)$; herein, values and formulations are the same as those used by Bolton (1980).

The code works as follows. Values of temperature are obtained using (14) as an air parcel is displaced vertically. Herein, pressure increments of 1 hPa are used. The mixing ratio of total water is conserved during this displacement. If vapor pressure, or e , is less than saturation vapor pressure, or e_s , after a displacement, then r_v is conserved ($dr_v = 0$). However, if e exceeds e_s during a vertical displacement, then saturated equilib-

rium is assumed and water is condensed such that $e = e_s$. An iterative procedure is used to determine the temperature that satisfies both (14) and the condition $e = e_s(T)$.

To obtain an exact pseudoadiabatic lapse rate, (14) is used and condensate is immediately removed after the completion of each vertical displacement. This is standard practice to obtain a pseudoadiabatic lapse rate. A comparison of output from this code with results reported by Bolton (1980, in his Table 3) shows that the code used herein produces essentially identical results; the maximum difference is 0.05 K.

To test the accuracy of the approximate equations developed in the previous section, a separate set of integrations are conducted in which condensed water is carried aloft during vertical displacements (as in a reversible process), but (10) is used as the governing equation (assuming $ds^p = 0$).

Results for a parcel starting at $p = 1000$ hPa and $T = 30^\circ\text{C}$ are shown in Fig. 2a, assuming $L_0 = 2.555 \times 10^6 \text{ J kg}^{-1}$. Two cases are shown in this figure. One case assumes that the initial parcel is saturated ($\mathcal{H} = 1$), which is the rightmost set of curves in Fig. 2a; in this case, temperature immediately follows a pseudoadiabatic lapse rate, and continues until all water is condensed. The second case assumes the initial parcel is subsaturated (with $\mathcal{H} = 0.5$), which is the leftmost set of curves in Fig. 2a; in this case, potential temperature is approximately conserved until the parcel cools to satu-

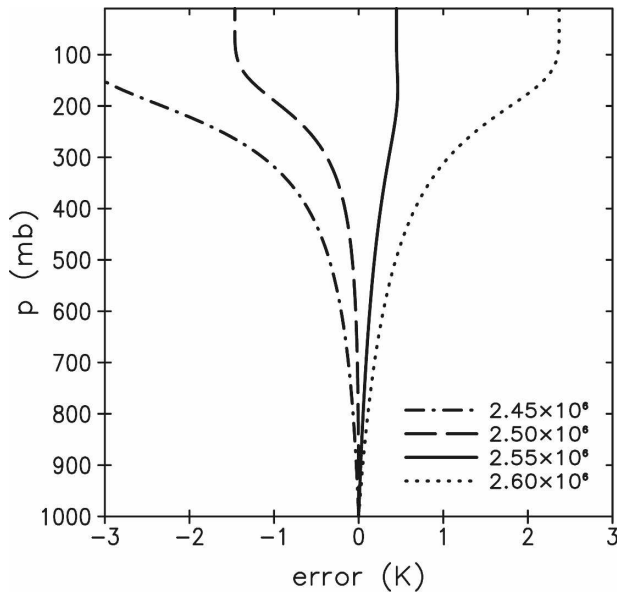


FIG. 3. Potential temperature errors using the approximate equation with different values for L_0 .

ration, and then a pseudoadiabatic lapse rate is followed. These two cases are shown to demonstrate that the approximate equation in (10) applies reasonably well to both subsaturated and saturated environments. In both cases, the approximate results (dashed lines in Fig. 2a) are good approximations to the exact results (solid lines in Fig. 2a). The potential temperature errors, shown in Fig. 2b, are always less than 0.6 K.

In the subsaturated case ($\mathcal{H} = 0.5$), the parcel using the approximate equation cools artificially (relative to the integration using the exact equation) during the first hundred hectopascals of ascent, owing to the neglect of ϵ_1 (i.e., owing to the neglect of the contribution of water vapor to entropy). Because of this slight relative cooling, this parcel reaches saturation earlier than the parcel using the exact equation. Then, the parcel using the approximate equation follows a saturated pseudoadiabatic while the parcel using the exact formulation cools further until saturation is achieved. The difference in saturation points is what accounts for the abrupt change in error at ~ 850 hPa.

This test has been repeated for different values of the initial pressure, temperature, and relative humidity. In all cases, results from the approximate equation are good approximations to results from the exact pseudoadiabatic formulation. In fact, the cases shown in Fig. 2 produce the largest errors from all of these tests.

The sensitivity to the value chosen for L_0 is illustrated in Fig. 3, assuming initial values $p = 1000$ hPa, $T = 30^\circ\text{C}$, and $\mathcal{H} = 1$. Obviously, the value chosen for L_0 has an effect on the accuracy of the solution. For

TABLE 1. Results from numerical evaluation of different formulations for θ_e^p , where p , T , and \mathcal{H} refer to the values of pressure, temperature, and relative humidity, respectively; θ_e^p refers to the value retrieved from the numerical code; δ_1 refers to the error of θ_e^p using Bolton's formulation (6); and δ_2 refers to the error of θ_e^p using the new formulation (13).

p (hPa)	T ($^\circ\text{C}$)	\mathcal{H}	θ_e^p (K)	δ_1 (K)	δ_2 (K)
1000	30	1	386.33	-0.04	0.40
1000	20	1	335.62	-0.03	0.14
1000	0	1	283.59	0.04	-0.06
1000	-30	1	244.01	0.01	-0.02
700	20	1	394.74	-0.07	0.05
700	0	1	319.13	0.03	-0.10
700	-30	1	270.57	0.02	-0.03
200	-30	1	391.82	0.03	-0.17
200	-50	1	354.12	0.00	-0.03
1000	30	0.5	344.31	-0.03	-0.39
1000	20	0.5	314.75	0.03	-0.26
1000	0	0.5	278.57	0.04	-0.11
1000	-30	0.5	243.60	0.01	-0.02
700	20	0.5	359.66	-0.01	-0.46
700	0	0.5	311.06	0.04	-0.17
700	-30	0.5	269.92	0.01	-0.02
200	-30	0.5	388.49	0.02	-0.12
200	-50	0.5	353.70	0.00	-0.02

$L_0 = 2.50 \times 10^6 \text{ J kg}^{-1}$ (the value valid at $T = 0^\circ\text{C}$, which is a commonly used constant value of L_0 in numerical models), results show a cold bias that becomes unacceptably large (1.5 K) at low pressures.

5. Evaluation of equivalent potential temperature

In this section, the new formulation for θ_e^p (13) is compared with Bolton's formulation (6). To this end, the numerical code is used to determine exact values of θ_e^p given specified values of p , T , and \mathcal{H} . Specifically, the value for θ_e^p is the value of θ at the end of the integration (herein, when the parcel reaches 10 hPa) when using the exact pseudoadiabatic formulation.

Results are listed in Table 1. Also listed are δ_1 , which is defined as the error when using Bolton's formula, and δ_2 , which is defined as the error when using the new formulation. In general, the new formulation produces larger errors than Bolton's formulation. However, even the largest error (~ 0.4 K), which occurs in very warm and moist environments, is acceptable for most applications.

As mentioned earlier, the value of L_0 is unconstrained in the new approximate equations, but an optimal value should be chosen such that $\epsilon_1 \approx \epsilon_2$ in most environments. To determine this optimal value, the tests shown in Table 1 were repeated with different values of L_0 until the mean-square error of all cases

listed in Table 1 was minimized. The value $L_0 = 2.555 \times 10^6 \text{ J kg}^{-1}$ produced the best result and therefore has been used for all results shown herein.

6. Summary

New approximate mathematical formulas for pseudo-adiabatic entropy, or s^p , and equivalent potential temperature, or θ_e^p , are derived herein. The primary assumptions are that the contribution to entropy from water vapor can be neglected (because $\epsilon_1 \approx 1$) and that the subsequent error can be compensated by using a constant value for the latent heat of vaporization (because $\epsilon_2 \approx 1$). These assumptions have been considered many times previously (e.g., Iribarne and Godson 1981). However, a further important conclusion that probably has not been presented previously is that L_0 can be assigned a value that ensures that these two assumptions have compensating errors (i.e., $\epsilon_1 \approx \epsilon_2$). Numerical evaluation herein has determined an optimal value of $L_0 = 2.555 \times 10^6 \text{ J kg}^{-1}$.

Further numerical evaluation herein demonstrates that the approximate thermodynamic equation in (10) can accurately reproduce the exact pseudoadiabatic process. Furthermore, consistent mathematical formulations are derived for pseudoadiabatic moist entropy, given by (11), and pseudoadiabatic equivalent potential temperature, given by (13). Most significant is that these formulations do not require expensive numerical integration (as do the exact equations for a pseudoadiabatic process), and were not derived using empirical fits to data [as was done by Bolton (1980)].

In tests with a numerical code, the new formulation of θ_e^p is found to have larger inherent errors when compared with the empirical formulation derived by Bolton

(1980), although the errors are acceptable ($<0.4 \text{ K}$) for most practical applications. Unlike Bolton's formulation, the new formulation has a consistent mathematical definition for s^p and a consistent first law of thermodynamics. Because these formulations are expressed in a convenient and simple physical form, they should be very useful for theoretical applications.

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