Another Look at the Thermodynamic Equation For Deep Convection

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ABSTRACT

The study considers deep moist convection involving only a liquid-vapor phase change. An alternative form of the classical thermodynamic equation for reversible saturated flow is derived. Four approximate forms of this equation are obtained and their relative errors compared to the full equation are evaluated by using parcel theory. The best approximation is found to be an adequate representation of the full equation throughout the total depth of the convection.

The two best approximations are compared with some forms of the thermodynamic equation used by other investigators.

1. Introduction

In this study the form of the thermodynamic equation used to represent deep moist convection is examined. The thermodynamics is assumed to be reversible and the equation obtained must be valid for both saturated and unsaturated conditions. It is realized that the assumption of reversibility is not valid for deep convection in the atmosphere. Such important non-reversible effects as turbulent diffusion and the formation, fallout and evaporation of finite raindrops are not included. What is of primary interest here is an accurate expression of reversible moist thermodynamics into which these non-reversible effects may be included as required in a given theoretical model.

At first glance it might appear that a discussion of such a basic thermodynamic equation would not be required. Indeed, a well-known classical expression of the reversible first law for moist convection is given by Eq. (1b). In this equation, the heating of the air is given in terms of the dry air potential temperature θ_d which is expressed in terms of the partial pressure p_d of the dry air. In theoretical models, however, the potential temperature θ, defined in terms of the total pressure p, is commonly used. It is when (1b) is replaced by an equation which involves θ instead of θ_d that various approximations are made and ambiguities arise.

A recent discussion of the thermodynamic equation for saturated adiabatic flow has been given by Wilhelmson (1977). Various approximations of the first law are compared with Eq. (1b) and the resulting differences in θ_d are computed as functions of p_d for three different cloud base heights. His analysis, however, contains various approximations. The latent heat of vaporization l_v in Eq. (1b) is given the

constant value $l_v = 2.500 \times 10^6$ J kg^{-1}. Since in reality l_v varies slowly with temperature, there is some error in the calculated comparisons. Another major ambiguity of his analysis is that Wilhelmson does not clearly distinguish between θ and θ_d or between p and p_d. For the comparisons in his study, the differences between θ_d as calculated from (1b) and from the other approximate forms of the first law are often several degrees or more. When such large differences exist, Wilhelmson's approximations are probably a relatively small source of error.

In the present study we consider different forms of the thermodynamic equation which have relative errors $\leqslant 0.5$ K. This degree of accuracy is considered necessary to represent atmospheric situations in which the temperature excess in the cloud may be only a few degrees warmer than the surrounding atmosphere. For this accuracy a clear distinction between θ and θ_d and between p and p_d must be made in all expressions. In addition, the importance of the variation of l_v with temperature must be evaluated. In Section 2 an exact alternative equation to (1b) is derived which involves θ instead of θ_d. Approximations to this exact equation are made in Section 3a and their relative errors are discussed. In Section 3b a comparison is made between the present approximate equations and some forms of the thermodynamic equation used by other researchers.

2. Derivation of alternative form of the thermodynamic equation

a. Saturated adiabatic flow

A standard form of the equation for reversible saturated motion is given by Iribarne and Godson (1973, Chap. 6) as

$$[c_{pd} + c_w(r_s + w)]d \ln T$$
$$- R_d d \ln p_d + d(l_v r_s/T) = 0, \quad (1a)$$

where T is the temperature, p_d the partial pressure of the dry air, r_s the saturation value of the water vapor mixing ratio, w the cloud water mixing ratio, l_v the latent heat of vaporization, c_{pd} the specific heat of dry air at constant pressure, c_w the specific heat of liquid water and R_d the gas constant for dry air. A well-known equivalent form of this equation is

$$c_{pd}d \ln\theta_d + c_w(r_s + w)d \ln T + d(l_v r_s/T) = 0, \quad (1b)$$

where θ_d is the potential temperature of the dry air.

In this study an alternative form of (1b) will be obtained in which θ_d is replaced by the potential temperature θ. These two quantities are defined by

$$\theta_d = T\left(\frac{P_0}{p_d}\right)^\kappa, \quad \theta = T\left(\frac{P_0}{p}\right)^\kappa, \quad \kappa = R_d/c_{pd}, \quad (2)$$

where p is the total pressure of the moist air and P_0 is a reference pressure level. To obtain the alternative form of (1b), in addition to reversibility and saturation, three explicit assumptions are made: (i) water vapor and dry air behave as perfect gases; (ii) the coefficients c_{pd}, c_{pv}, R_d, R_v and c_w are constant and l_v is a linear function of T; and (iii) the specific volume of liquid water is neglected in the Clausius-Clapeyron equation. Using assumption (i), r_s is given by

$$r_s = \frac{R_d}{R_v}\frac{e_s}{p_d}, \quad (3)$$

where e_s is the saturation vapor pressure and R_v is the gas constant for water vapor. Likewise, using assumptions (ii) and (iii), Kirchhoff's law and the Clausius-Clapeyron equation are given by

$$\frac{dl_v}{dT} = c_{pv} - c_w \quad (4)$$

and

$$\frac{d \ln e_s}{dT} = \frac{l_v}{R_v T^2}, \quad (5)$$

where c_{pv} is the specific heat of water vapor at constant pressure.

Now, using (4) and (5), Eq. (1a) can be written as

$$(c_{pd} + c_{pv}r_s + c_w w)d \ln T - R_d d \ln p_d$$
$$- R_v r_s d \ln e_s + \frac{l_v}{T} dr_s = 0. \quad (6)$$

Likewise using (3) and the relation $p = p_d + e_s$ for the total pressure, Eq. (6) can be put in the form

$$c_{pd}\left(1 + \frac{c_{pv}}{c_{pd}}r_s\right)d \ln T - R_d\left(1 + \frac{R_v}{R_d}r_s\right)d \ln p$$
$$= -\frac{l_v}{T} dr_s - c_w w d \ln T. \quad (7)$$

It is remarked that this last equation is equivalent to the result given in Section 3.32 of Holmboe, et al. (1945). Finally, using the definition of θ and dividing by $[1 + (R_v/R_d)r_s]$, Eq. (7) can be written as

$$c_{pd}d \ln\theta = -\left(1 + \frac{R_v}{R_d}r_s\right)^{-1}\left\{\frac{l_v}{T} dr_s\right.$$
$$\left. + \left[c_w w + c_{pd}r_s\left(\frac{c_{pv}}{c_{pd}} - \frac{R_v}{R_d}\right)\right]d \ln T\right\}. \quad (8)$$

Eq. (8) is considered as the alternative to (1b) in the present study. To the authors' knowledge, this equation represents the first time that the reversible moist adiabatic thermodynamic equation has appeared in this form in the meteorological literature.

b. Unsaturated adiabatic flow

In unsaturated adiabatic motion the liquid water mixing ratio w is zero and the water vapor mixing ratio r is conserved following a parcel. Thus, for the parcel, the thermodynamics can be treated as for an ideal gas with fixed ratios of constituents

$$c_{pd}\left(1 + \frac{c_{pv}}{c_{pd}}r\right)d \ln\theta_m = 0, \quad (9)$$

where

$$\theta_m = T\left(\frac{P_0}{p}\right)^{\kappa(r)}, \quad \kappa(r) = \frac{R_d}{c_{pd}}\frac{\left(1 + \frac{R_v}{R_d}r\right)}{\left(1 + \frac{c_{pv}}{c_{pd}}r\right)}. \quad (10)$$

These expressions for the moist potential temperature θ_m and $\kappa(r)$ are equivalent to those given by Iribarne and Godson (1973, Chap. 4). These authors also find that the difference $(\theta_m - \theta)$ is very small, being generally less than 0.1 K. Hence, to a high degree of accuracy, the potential temperature θ is conserved for unsaturated reversible flow.

It can be seen that Eq. (9) is equivalent to Eq. (7) with $w = 0$ and $dr_s = 0$, and is therefore equivalent to Eq. (8) under the same conditions. Thus Eq. (8) can be considered the exact equation for reversible adiabatic flow whether saturated or unsaturated. Likewise, the approximate equations (11) and (13a)–(13c) obtained below reduce to $c_{pd}d \ln\theta = 0$ when $w = 0$ and $dr_s = 0$. Thus they also can be considered as approximate equations representing both saturated and unsaturated flow.

3. Approximate forms of the thermodynamic equation

a. Approximate forms of Eq. (8)

Several approximate forms of Eq. (8) are now considered. The most accurate of these is given by

$$c_{pd}d \ln\theta = \left(1 + \frac{R_v}{R_d}r_s\right)^{-1}\left(-\frac{l_v}{T}dr_s\right) - c_w wd \ln T, \quad (11)$$

where the temperature dependence of l_v is retained. Compared with (8), it is seen that the last term, $c_{pd}r_s[(c_{pv}/c_{pd}) - (R_v/R_d)]d \ln T$, on the right side of (8) has been dropped. The factor $[1 + (R_v/R_d)r_s]^{-1}$ multiplying $(-c_w wd \ln T)$ has also been set equal to unity. The relative magnitudes of these two approximations will be estimated below.

The dominant term on the right side of (8) is the latent heating term which is represented by $(l_v/T)dr_s$ inside the large parentheses. The magnitudes of the two approximations used to obtain (11) will be compared with the estimated magnitude of the $(l_v/T)dr_s$ term. This latent heating term is labeled as A and its magnitude is estimated by considering that the major variation in dr_s is due to the variation of the saturation vapor pressure e_s. Using (3) and (5) we find

$$A = \frac{l_v}{T}dr_s \approx \frac{l_v}{T}\frac{l_v r_s}{R_v T}d \ln T. \quad (12a)$$

The last term on the right side of (8) is labeled C and can be approximated[1] by

$$C = c_{pd}r_s\left(\frac{c_{pv}}{c_{pd}} - \frac{R_v}{R_d}\right)d \ln T$$

$$\approx \frac{1}{7}c_{pd}\frac{R_v}{R_d}r_s d \ln T. \quad (12b)$$

When the factor $[1 + (R_v/R_d)r_s]^{-1}$ multiplying the $-c_w wd \ln T$ term in (8) is dropped, we are in effect neglecting the term

$$B = \frac{\frac{R_v}{R_d}r_s}{1 + \frac{R_v}{R_d}r_s} c_w wd \ln T \approx \frac{R_v}{R_d}r_s c_w wd \ln T. \quad (12c)$$

The denominator in this expression is nearly equal to unity since $r_s \approx 10^{-2}$ and $R_v/R_d \approx 1.6$. The values of the various constant coefficients in the present study are given in the Appendix.

The relative magnitudes of the two terms neglected in Eq. (11) are now estimated from the ratios C/A and B/A. For atmospheric values of T we find

$$\frac{C}{A} \approx \frac{1}{7}c_{pd}\frac{R_v}{R_d}\bigg/\left(\frac{l_v}{T}\frac{l_v}{R_v T}\right) \approx 1.4 \times 10^{-3}, \quad (12d)$$

$$\frac{B}{A} \approx c_w\frac{R_v}{R_d}w\bigg/\left(\frac{l_v}{T}\frac{l_v}{R_v T}\right) \approx 0.4 \times 10^{-3}, \quad (12e)$$

where $w \approx 10^{-2}$ is assumed in (12e). Thus the present analysis finds that the terms neglected in (11) appear to be negligible when compared with the latent heating term.

A larger approximation is made when the factor $[1 + (R_v/R_d)r_s]^{-1}$ multiplying $[-(l_v/T)r_s]$ is set equal to unity. It can be seen that neglecting this factor represents the relative error $(R_v/R_d)r_s \approx 1.6 \times 10^{-2}$ with respect to the total term $-[1 + (R_v/R_d)r_s]^{-1} \times (l_v/T)dr_s$. This additional approximation leads to the equation

$$c_{pd}d \ln\theta = -\frac{l_v}{T}dr_s - c_w wd \ln T. \quad (13)$$

The importance of the variation of l_v with temperature will be examined for this equation. Thus three forms of (13) are considered:

$$l_v = \begin{cases} l_v(T) \text{ is a function of temperature} & (13a) \\ 2.5 \times 10^6 \text{ (J kg}^{-1}\text{)}, \quad T \approx 273 \text{ K} & (13b) \\ l_v(T_0), T_0 = \text{temperature at cloud base} & (13c) \end{cases}$$

Note that for both (13b) and (13c), l_v is held constant. The relative accuracy of (11) and (13a)–(13c) compared with the full equation (8) will be examined from parcel theory.

The saturation parcel calculations are carried out in a manner similar to Wilhelmson (1977). The saturation mixing ratio r_s is given by (3). The saturation vapor pressure $e_s(T)$ is calculated from the Clausius-Clapeyron equation (5) using the assumption that l_v is a linear function of temperature, i.e.,

$$l_v = l_1 - l_2 T, \quad (14)$$

so that

$$e_s(T) = e_s(T_0)$$

$$\times \exp\left\{\frac{1}{R_v}\left[l_1\left(\frac{T - T_0}{TT_0}\right) - l_2 \ln\left(\frac{T}{T_0}\right)\right]\right\}, \quad (15)$$

where $e_s(T_0)$ is the saturation vapor pressure at cloud base. Here the constants l_1 and l_2 have been chosen to give a good fit to l_v for temperatures at and above the freezing point of water. It is also a reasonable fit for lower temperatures as well. We find that Eq. (15) is of comparable accuracy as

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[1] Air is primarily a diatomic gas so that $c_{pd}/R_d \approx 7/2$, whereas water vapor is a triatomic gas so that $c_{pv}/R_v \approx 4$. These two ratios imply $(c_{pv}/c_{pd}) - (R_v/R_d) \approx \frac{1}{7}(R_v/R_d)$.

Tetens' formula for temperatures encountered near and above cloud base.

The parcel calculations require a relationship between $d \ln\theta$ and $d \ln\theta_d$. From Eqs. (2) and, (3) and the relation $p = p_d + e_s$ we find

$$c_{pd}d \ln\theta = c_{pd}d \ln\theta_d$$

$$- R_v dr_s \left(1 + \frac{R_v}{R_d} r_s \right)^{-1} . \quad (16)$$

Using (2), (3), (15) and (16), the potential temperature θ_d can be calculated as a function of p_d from cloud base upward for Eqs. (8), (11) and (13a)–(13c). The temperature is expressed in terms of θ_d and p_d from the definition of θ_d in (2). The solutions for θ_d, T and r_s as functions of p_d are calculated using an iterative technique. As in Wilhelmson (1977), an increment of 10 mb is used in numerically integrating the above equations. Potential temperature differences for $i = (11)$, (13a)–(13c) corresponding to Eqs. (11), (13a)–(13c) have been calculated using (8) as the reference value of θ_d, i.e.,

$$(\Delta\theta_d)_i = (\theta_d)_i - (\theta_d)_8. \quad (17)$$

Calculations were also carried out using Eq. (1b). Potential temperature differences $(\Delta\theta_d)_{1b}$ between the values of θ_d for (1b) and (8) were negligible. Thus, as expected, Eqs. (1b) and (8) are equivalent.

The present study considers two sets of calculations, the first corresponding to one of the cases considered by Wilhelmson (1977) with cloud base at $p_d = 900$ mb, $T_0 = 284.3$ K, $\theta_d = 293$ K and $r_s = 0.917 \times 10^{-2}$. This is case I with the (relatively) cold, high cloud base. Case II (warm cloud base) has $p_d = 920$ mb, $T_0 = 293.9$ K, $\theta_d = 301$ K and $r_s = 1.657 \times 10^{-2}$ at cloud base. Results for both cases are shown in Fig. 1. The vertical dashed lines show the temperatures 0, −20 and −40°C as calculated from (8). Because of the presence of ice in observed clouds, the present results are considered to have limited relevance for temperatures between −20 and −40°C and little relevance for temperatures colder than −40°C. The calculations are stopped at $p_d = 300$ mb for case I and at $p_d = 200$ mb for case II.
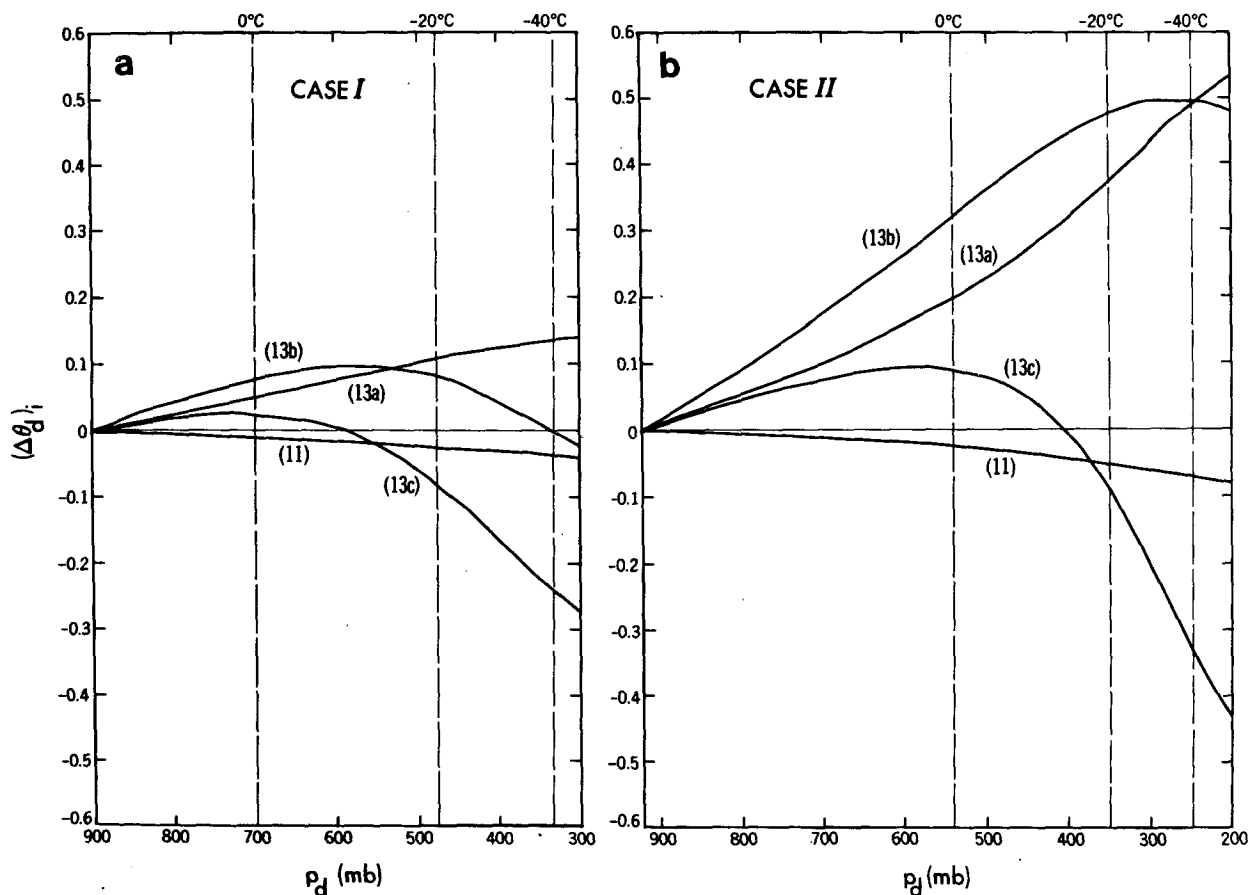

FIG. 1. Dry air potential temperature differences between parcel theory calculations using Eqs. (11) and (13a)–(13c), and Eq. (8).
Fig. 1a represents case I with the cold cloud base at $p_d = 900$ mb and 1b represents case II with the warm cloud base at $p_d = 920$ mb.

The data shown in Fig. 1 indicate that Eq. (11) is a very accurate approximation to the full equation (8). For both case I and case II, Eq. (11) represents a slow monotonic relative cooling with height. For a cloud parcel temperature of $-20°C$, case I has $\Delta\theta_d = -0.026$ K and Case II has $\Delta\theta_d = -0.051$ K. At a cloud temperature of $-40°C$, case I has $\Delta\theta_d = -0.037$ K and case II has $\Delta\theta_d = -0.070$ K. These small values of $\Delta\theta_d$ give conclusive evidence that, as indicated by (12d) and (12e), the terms neglected in (11) are negligible. Thus (11) is an adequate approximation to (8).

The curves for (13a)–(13c) are also shown in Fig. 1. For temperatures warmer than $-20°C$, these curves indicate that (13c) is the best approximation to (8) of the three cases. In this temperature range, it is seen that (13c) is an excellent approximation to (8) with $|\Delta\theta_d| < 0.1$ K. For colder temperatures, the data in Fig. 1 indicate that (13b) gives the best approximation for case I and that (13c) continues to give the best approximation for case II. Over the total temperature range, it is evident that (13c) gives the best representation of (8).

b. Other approximate forms of the thermodynamic equation

The above approximations to Eq. (8) are compared with other forms of the thermodynamic equation used by different researchers. The first equation considered is that given by Das (1969):

$$c_{pd}d \ln\theta_d + (l_v/T)dr_s = 0, \qquad (18)$$

where l_v is assumed to remain constant. Das (1969) argued that (18) was an accurate representation of the thermodynamics to within 10%. After comparing various forms of the thermodynamic equation, Wilhelmson (1977) concluded that (18) represents a good approximation to (1b) for deep saturated thermodynamics. For the present calculations l_v is set equal to $l_v = 2.500 \times 10^6$ J kg^{-1} which is the same value as used in (13b) and is the value used by Wilhelmson (1977).

The second form of the thermodynamic equation considered is given by

$$\frac{d\theta}{\Theta} + \frac{l_v}{c_{pd}T_{00}} dr_s = -\frac{c_w}{c_{pd}T_{00}} wdT, \qquad (19)$$

where Θ and T_{00} are constant reference values of the potential temperature and temperature, respectively. Eq. (19) is similar to a simplified form of the thermodynamic equation used by Orville and Kopp (1977) obtained when the effects of diffusion, finite size raindrops and freezing are neglected in their Eq. (30). Orville and Kopp, however, do not retain the full term involving dT on the right side of (19). Their thermodynamic equation includes the effect of heating due to the advection of cloud water

but does not include the corresponding heating associated with the local time derivative of temperature. In this respect (19) is slightly more general than their equation.

Eq. (19) can be written in the form

$$c_{pd}d \ln\theta = -\frac{1}{\pi_{00}\theta} (l_vdr_s + c_wwdT), \qquad (20)$$

where $\pi_{00} = T_{00}/\Theta$. From Eq. (2), θ can be defined by the relation $T = \pi\theta$ where the pressure function π is given by

$$\pi = \left(\frac{p}{p_0}\right)^\kappa, \quad \kappa = R_d/c_{pd}. \qquad (21)$$

Thus π_{00} can be considered as a reference value of π. In the present calculations π_{00} is set equal to $\pi_{00} = 0.903$, corresponding to a pressure $p = 700$ mb. The latent heat of vaporization is again held constant at the value $l_v = 2.500 \times 10^6$ J kg^{-1}.

A comparison of the curves obtained from parcel theory for (18) and (20) with those obtained for (11) and (13c) is given in Fig. 2, where Fig. 2a represents case I (cold cloud base) and Fig. 2b represents case II (warm cloud base). It can be seen that (11) and (13c) represent much better approximations to Eq. (8) than either (18) or (20). A possible modification in the calculations for (18) and (20) is to set l_v equal to $l_v(T_0)$, where T_0 is the temperature at the cloud base. Such a modification for (18) and (20) for both case I and case II results in smaller values of the positive deviations $(\Delta\theta_d)_i$ but it also results in larger negative deviations at the higher levels (lower p_d). Thus, using $l_v = l_v(T_0)$ does not result in a significant improvement in the approximate equations (18) and (20).

An alternative form of Eq. (18) for which θ_d is replaced by θ is shown by the curves labeled W in Fig. 2. The reason for plotting these curves is that this form of (18) appears to correspond to the thermodynamic equation used by Wilhelmson and Ogura (1972), Wilhelmson (1974) and Klemp and Wilhelmson (1978a,b). It should be also noted that these curves correspond to Eq. (13b) with the liquid water heating term, $-c_wwd \ln T$, neglected. As seen in Fig. 2, the curves using θ in (18) are much more accurate for temperatures warmer than $-10°C$, being comparable in accuracy to (13c). For colder temperatures, however, these curves indicate a rapidly increasing negative temperature difference compared with (8).

4. Summary and conclusions

Eq. (8) has been obtained as an alternative to Eq. (1b) for saturated reversible thermodynamics. This equation is expressed in terms of the potential temperature θ instead of the dry air potential tem-
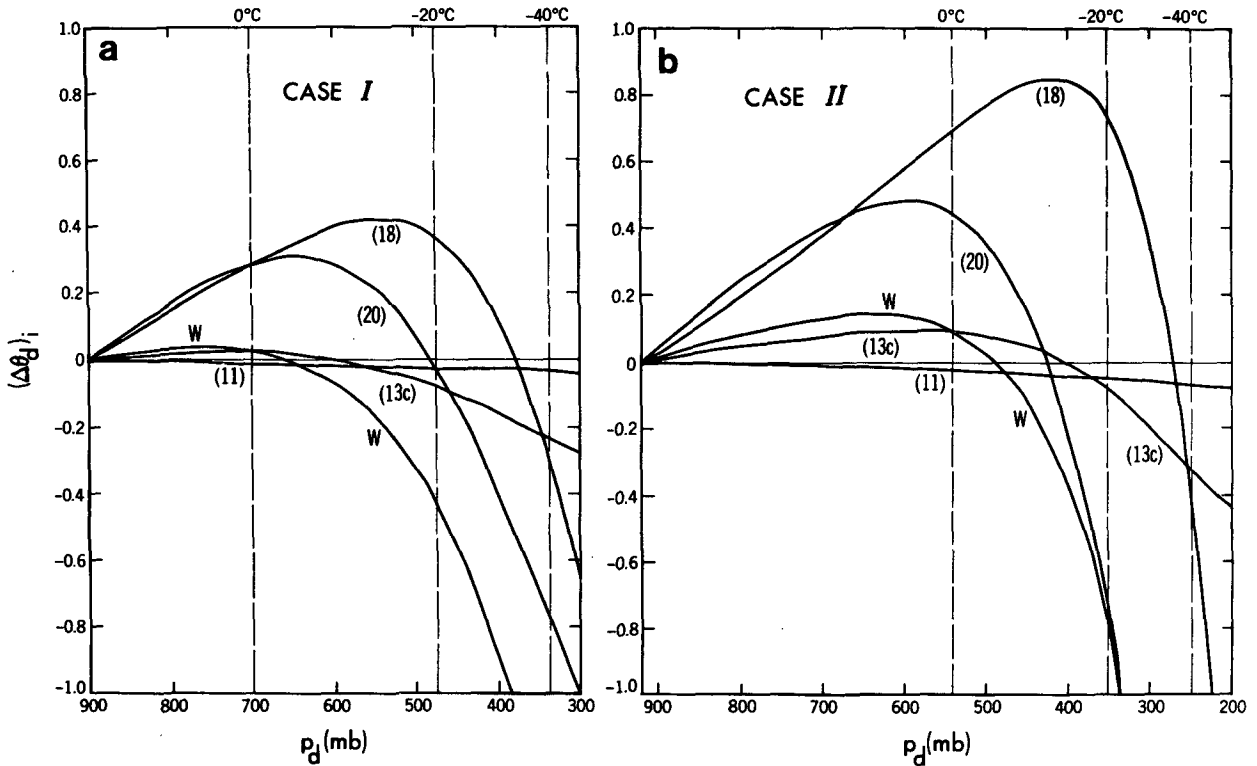
FIG. 2. Dry air potential temperature differences between parcel theory calculations using Eqs. (18), (20), (11) and (13c), and Eq. (8). The curve-marked W indicates Eq. (18) but with θ_d replaced by θ. As previously, Figs. 2a and 2b are for cloud base at $p_d = 900$ mb and $p_d = 920$ mb, respectively.

perature θ_d and has been derived subject to the three assumptions listed in Section 2a. Approximations to (8) are given as Eqs. (11) and (13a)–(13c). The discussion in Section 2b indicates that Eqs. (8), (11) and (13a)–(13c) can also be applied to the unsaturated reversible case.

The accuracy of (11) and (13a)–(13c) compared with (8) is evaluated in Section 3a by using parcel theory. The results are shown in Fig. 1. The most accurate approximation is Eq. (11) with the difference in values of θ_d for (8) and (11) being less than 0.1 K for all p_d. This small difference between (8) and (11) is sufficient reason to consider (11) as an adequate approximation to (8). Of the three cases (13a)–(13c), Eq. (13c) gives the best approximation to (8). For a problem which involves warm clouds only, (13c) is thought to be sufficiently accurate.

If the ice phase is included in deep convection, a variable $l_v(T)$ is probably required for an accurate representation of the thermodynamics. When freezing occurs, the relation $l_s = l_f + l_v$ should be satisfied. In this expression the latent heat of sublimation l_s is approximately constant whereas the latent heats of fusion and vaporization, l_f and l_v, are variables. For this case Eq. (11) can be used to represent the thermodynamics before freezing occurs. This conclusion is in agreement with the study of Orville and Hubbard (1973) who found

that variations in l_v and l_f can be important in the thermodynamics of deep convection.

The accuracy of other approximate forms of the thermodynamic equation is discussed in Section 3b. Two of these equations are the equation suggested by Das (1969) and an equation representing the thermodynamic approximation used by Orville and Kopp (1977). In the text, these two equations are given by (18) and (20), respectively. These two approximations are compared against Eqs. (11) and (13c) in Fig. 2. It is seen that both (11) and (13c) represent much better approximations to the exact equation (8) than either (18) or (20). The curves labeled W in Fig. 2 represent an alternative form of (18) for which θ_d is replaced by θ. It is seen that this form of (18) is much more accurate than Das' equation, being comparable in accuracy to (13c) for temperatures warmer than $-10°C$. This last comparison shows that the difference between using θ and θ_d is significant for the accuracy of the present study.

APPENDIX

Numerical Values of Constant Coefficients

c_{pd} specific heat of dry air at constant pressure (1005.7 J kg^{-1} K^{-1})

c_{pv} specific heat of water vapor at constant pressure (1860.6 J kg^{-1} K^{-1})

R_d gas constant for dry air (287.04 J kg^{-1} K^{-1})

R_v gas constant for water vapor (461.50 J kg^{-1} K^{-1})

$$\left(\frac{c_{pv}}{c_{pd}} - \frac{R_v}{R_d} \right) = 0.2423$$

P_0 reference pressure level (1000 mb)

c_w specific heat of water (4217.8 J kg^{-1} K^{-1})

l_1 constant in Eq. (16) for l_v (3.1447 $\times$ 10^6 J kg^{-1})

l_2 constant in Eq. (16) for l_v (2357.2 J kg^{-1} K^{-1})

$$\left[= -\frac{dl_v}{dT} \right]$$

Note that c_{pv}, c_w and dl_v/dT have been required to be compatible with Kirchhoff's law [$dl_v/dT = c_{pv} - c_w$].

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