The Use of Ice-Liquid Water Potential Temperature as a Thermodynamic Variable in Deep Atmospheric Models

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(Manuscript received 8 May 1980, in final form 4 February 1981)

ABSTRACT

Previous studies have shown liquid water potential temperature to be an inappropriate choice for a thermodynamic variable in a deep cumulus convection model. In this study, an alternate form of this variable called ice-liquid water potential temperature (θ_{il}) is derived. Errors resulting from approximations made are discussed, and an empirical form of the θ_{il} equation is introduced which eliminates much of this error. Potential temperature lapse rates determined in saturated updrafts and unsaturated downdrafts by various θ_{il} approximations, an equivalent potential temperature approximation and a conventional irreversible moist thermodynamic approximation are then compared to the potential temperature lapse rate determined from a rigorously derived reversible thermodynamic energy equation. These approximations are then extended to a precipitating system where comparisons are again made. It is found that the errors using the empirical form of the θ_{il} equation are comparable to those made using conventional irreversible moist thermodynamic approximations. The advantages of using θ_{il} as an alternative to θ in deep convection and second-order closure models also are discussed.

1. Introduction

Liquid water potential temperature (θ_L) was first introduced by Betts (1973) as a conservative thermodynamic variable for non-precipitating convection. Later, Deardorff (1976), and Sommeria and Deardorff (1977) successfully incorporated it into a three-dimensional shallow convection model using subgrid-scale turbulence closure. The variable θ_L is found particularly useful for turbulent closure models because it is conserved for liquid to vapor phase changes, while it becomes synonymous with potential temperature θ when no liquid water is present. Its use was extended to a set of precipitating, deep convection equations using second-order turbulence closure by Manton and Cotton.[1] Wilhelmson (1977), however, demonstrated that application of θ_L to deep convection produced very large positive temperature errors when compared to reversible moist ascent over the depth of the troposphere.

In this work, the derivation of θ_L is reexamined in order to gain insight into which approximations lead to the errors in θ_L that Wilhelmson (1977) pointed out. Also, the ice phase is added and new approximate formulas are derived defining ice-liquid water potential temperature (θ_{il}). The variable θ_{il}

is conservative under vapor to liquid, vapor to ice and liquid to ice phase changes. These formulations are then empirically modified to closely fit temperature variations given by a more rigorous form of the first law. A description of the performance of θ_{il} compared to some other thermodynamic approximations for moist ascent and subsaturated evaporative descent is given.

2. A rigorous form of the thermodynamic energy equation

In a study of this type, a rigorously derived form of the thermodynamic energy equation must be selected as a norm or standard for which all more approximate forms of the thermodynamic energy equation can be compared. We begin with the first law of thermodynamics for open systems as developed by Dutton (1976) in the form (see Appendix for list of symbols)

$$d(C_p \ln T) - d(R \ln p_d) + d\left(r_v \frac{L_{lv}}{T}\right) - d_i\left(r_i \frac{L_{il}}{T}\right)$$
$$+ r_v d\left(\frac{A_{lv}}{T}\right) - r_i d\left(\frac{A_{il}}{T}\right) + rC_l d \ln T = 0. \quad (1)$$

Eq. (1) and subsequent equations in this paper will use a derivative notation presented by Dutton (1976). The subscript i following a derivative operator refers to changes in a quantity occurring internally within the parcel. The subscript e (for ex-

[1] Manton, M. J., and W. R. Cotton, 1977: Formulation of approximate equations for modeling moist deep convection on the mesoscale. Atmos. Sci. Pap. No. 266, Colorado State University, NSF Grant DES 7513310, 62 pp.

ternal) following the derivative operator refers to changes in a quantity due to a net flux of that quantity into or out of the parcel. No subscript following the derivative operator refers to the total change which is the sum of the external and internal changes. Extensive variables can have external and internal derivatives if a flux of that quantity relative to the air parcel occurs. Intensive variables such as temperature, however, have external derivatives identically zero. As with Dutton (1976), we require vapor to move with the air parcel, i.e., $d_e r_v = 0$. In the case of (1), we therefore can see on inspection that the external variation in r_i will not influence the temperature change. On the other hand, the internal change of r_i must be due to a phase change and therefore will influence temperature. In the case of (1), sensible heat transport by precipitation into the parcel is neglected.

Eq. (1) is the same as the norm used in the study by Wilhelmson (1977) if (i) the ice phase is neglected, (ii) thermodynamic equilibrium over a plane surface of water is assumed (this implies r_v must vary as r_{vs}) and (iii) variations of R and C_p are neglected. In this study, we also will make assumption (iii), however, we will consider the ice phase and equilibrium will not be assumed. Instead, the affinity terms may be expressed as

$$A_{lv} = \mu_l - \mu_v \qquad (2)$$

and

$$A_{il} = \mu_i - \mu_l, \qquad (3)$$

where μ_v, μ_l and μ_i are the chemical potential of vapor, ice and liquid water. Following Fletcher (1962), the chemical potential of vapor may be defined as

$$\mu_v = \mu_0 + R_v T \ln e_v, \qquad (4)$$

where μ_0 is a base state chemical potential. The chemical potentials at the surface of the water droplet and ice particle are expressed by the equilibrium values of the vapor chemical potential at those surfaces. These chemical potentials may be expressed as

$$\mu_l = \mu_0 + R_v T \ln e_{sv} \qquad (5)$$

and

$$\mu_i = \mu_0 + R_v T \ln e_{si}. \qquad (6)$$

Strictly speaking, e_{sv} and e_{si} represent the saturated vapor pressures with respect to liquid and ice at the surface of individual drops and ice particles having surface temperatures differing from the ambient temperature T. We will ignore surface curvature and solution effects, however, and evaluate e_{sv} and e_{si} with respect to plane, pure water or ice surfaces at the ambient temperature T. From the equation of state, the identity

$$r_v R_v d \ln e_v = (R + r_v R_v) d \ln p - R d \ln p_d \qquad (7)$$

may be derived. Combining (1)–(7) and using the relationships

$$\frac{d}{dt} L_{lv} = C_{vp} - C_l, \qquad (8)$$

$$\frac{d}{dt} L_{il} = C_l - C_i, \qquad (9)$$

$$L_{il} = L_{iv} - L_{lv}, \qquad (10)$$

the first law may be rewritten as

$$C_{pm} d \ln T - R_m d \ln p + \frac{L_{lv}}{T} dr_v - \frac{L_{il}}{T} d_i r_i$$
$$+ (r_v + r_i)\left[L_{lv} d\left(\frac{1}{T}\right) + R_v d \ln e_{sv} \right]$$
$$- r_i \left[L_{iv} d\left(\frac{1}{T}\right) + R_v d \ln e_{si} \right] = 0, \qquad (11)$$

where $C_{pm} = C_p + r_v C_{vp} + r_i C_i + r_l C_l$ and $R_m = R + r_v R_v$.

Defining the variation in saturation vapor pressures from the Clausius-Clapeyron relation yields the value of zero for both bracketed terms. The final rigorous form of the first law is then

$$C_{pm} d \ln T - R_m d \ln p + \frac{L_{lv}}{T} dr_v - \frac{L_{il}}{T} d_i r_i = 0. \qquad (12)$$

This equation is similar to that used by Betts (1973) except that an ice term is included and equilibrium is not assumed. Since we have not assumed equilibrium, changes in r_v may or may not be the same as changes in saturation vapor pressure. As a result, this formulation should be more valid for subsaturated evaporation of liquid or ice water, supersaturated growth of ice, and other phase changes which may or may not be equilibrium processes. Because of this, (12) may not be reversible. For example, condensation during saturated ascent followed by evaporation in a subsaturated downdraft would not be a reversible process.

From Poisson's equation, potential temperature may be defined as

$$d \ln\theta = d \ln T - \frac{R}{C_p} d \ln p. \qquad (13)$$

Combining (13) with (12), we can write

$$d \ln\theta = \left(\frac{R_m}{C_{pm}} - \frac{R}{C_p} \right) d \ln p$$
$$- \frac{L_{lv}}{C_{pm} T} dr_v + \frac{L_{il}}{C_{pm} T} d_i r_i. \qquad (14)$$

In this study, we will use (14) as a norm for assessing the magnitude of errors associated with more approximate forms of the thermodynamic energy equation when it is applied to deep, moist convection.

An assumption used to simplify (14) is to neglect

the heat storage by water. As a result, (14) may be approximated by

$$d \ln\theta = -\frac{L_{lv}}{C_p T} dr_v + \frac{L_{il}}{C_p T} d_i r_i. \quad (15)$$

If equilibrium is assumed, then $dr_v = dr_{vs}$ and (15) becomes the classical moist pseudoadiabatic relationship, except for the additional ice term. This form is common to most deep atmospheric models.

Assuming conservation of total water given by

$$dr_v + d_i r_l + d_i r_i = 0, \quad (16)$$

and applying (10), we may rewrite (15) as

$$d \ln\theta = \frac{L_{lv}}{C_p T} d_i r_l + \frac{L_{iv}}{C_p T} d_i r_i. \quad (17)$$

Variations in θ given by (14), (15) and (17) occur only due to internal changes of r_i or r_l. Therefore, it is evident that changes in r_l and r_i due to precipitation will not affect θ. This, however, is not to say that (14), (15) or (17) are invalid for a precipitating system.

Because it is often desirable to obtain a thermodynamic variable which is conservative under adiabatic liquid and ice transformations, the ice-liquid water potential temperature is defined from (17) by

$$d_i \ln\theta_{il} = d \ln\theta - \frac{L_{lv}}{C_p T} d_i r_l - \frac{L_{iv}}{C_p T} d_i r_i = 0. \quad (18)$$

This definition is similar to that first proposed by Betts (1973) except for the ice phase term and lack of an equilibrium assumption. It should be noted that because θ_{il} is defined both by θ which is an intensive property and r_l and r_i which are extensive properties, θ_{il} too is extensive. Therefore, external fluxes of θ_{il} may occur into and out of the parcel due to relative precipitation movement. From (18), we know θ_{il} will be conserved provided all condensate remains within the original parcel. In the case that precipitation does occur, external fluxes of r_l and r_i and therefore θ_{il} must be taken into account when calculating the total change in θ_{il}. We will consider these changes more conveniently later in this section.

Similarly, an equivalent ice-vapor water potential temperature can be defined from (15) by

$$d_i \ln\theta_{eiv} \equiv d \ln\theta + \frac{L_{lv}}{C_p T} dr_v - \frac{L_{il}}{C_p T} d_i r_i = 0, \quad (19)$$

where θ_{eiv} is similar to the equivalent potential temperature except again for the ice phase term and the lack of an equilibrium requirement. As with the definition of θ_{il}, (19) refers only to internal changes in θ_{eiv}. This means θ_{eiv} is conservative over phase changes but not over precipitation fluxes into and out of the parcel. Hence (18) and (19) define two variables, both of which are conserved over water phase changes. The variable θ_{il} is especially useful as a model variable because it is identical to θ when no condensate is present, and does not vary as condensate forms (so long as the condensate is carried along with the parcel). The variable θ_{eiv} is useful in diagnostic studies as a tracer because it varies much the same as the moist static energy (e.g., see Betts and Silva Dias, 1979; Grandia and Marwitz, 1975; Zipser, 1969).

In order to make (18)–(19) more integrable, L_{lv}, L_{iv}, L_{il}, C_p and T are brought into the differential. Eqs. (18) and (19) then become

$$d_i \ln(\theta_{il}/\theta) = -d_i \left[\frac{L_{lv} r_l}{C_p T} + \frac{L_{iv} r_i}{C_p T} \right] + \epsilon_1 + \epsilon_2, \quad (20)$$

$$d_i \ln(\theta_{eiv}/\theta) = +d_i \left[\frac{L_{lv} r_v}{C_p T} - \frac{L_{il} r_i}{C_p T} \right] + \epsilon_3 + \epsilon_4, \quad (21)$$

respectively, where

$$\epsilon_1 = \frac{r_l}{C_p} d\left(\frac{L_{lv}}{T}\right), \quad (22)$$

$$\epsilon_2 = \frac{r_i}{C_p} d\left(\frac{L_{iv}}{T}\right), \quad (23)$$

$$\epsilon_3 = -\frac{r_v}{C_p} d\left(\frac{L_{lv}}{T}\right), \quad (24)$$

$$\epsilon_4 = \frac{r_i}{C_p} d\left(\frac{L_{il}}{T}\right). \quad (25)$$

It is evident that $d(L_{lv}/T)$, $d(L_{iv}/T)$ and $d(L_{il}/T)$ are all proportional to $-dT/T^2$ which grows nonlinearly as temperature becomes small. From (8) we know L_{lv} increases with decreasing temperature. Therefore, ϵ_1 will increase nonlinearly with decreasing temperature in the presence of liquid water. The ϵ_3 error, however, is weighted by vapor rather than liquid water. This leads to a diminished importance of ϵ_3 as the temperature falls, and the saturation mixing ratio becomes small exponentially. Hence ϵ_1 will become increasingly large at small T, while ϵ_3 will first increase and then decrease back toward 0 as r_v goes to zero. Also it can be noted, the ϵ_3 error is of opposite sign to ϵ_1. This will lead to opposite signs in the error given by (20) to that of (21) in the presence of liquid water only. Because L_{iv} varies very little with T, ϵ_2 is dominated by the inverse temperature error which increases with decreasing temperature in the presence of r_i. From (9) we know L_{il} decreases with decreasing temperature linearly. This will tend to cancel the inverse temperature error at higher temperatures, but the effects of inverse temperature must dominate as the temperature becomes low enough. Therefore, as ϵ_3 diminishes at low temperatures, the sign of the total error for (21) may reverse when ice is present and vapor is very small.

If we neglect ϵ_1, ϵ_2, ϵ_3 and ϵ_4, as is customary, we obtain the approximations

$$\theta_{il} = \theta \exp\left\{-\left[\frac{L_{lv}(T_0)r_l}{C_pT} + \frac{L_{iv}(T_0)r_i}{C_pT}\right]\right\}, \quad (26)$$

$$\theta_{eiv} = \theta \exp\left\{-\left[-\frac{L_{lv}(T_0)r_v}{C_pT} + \frac{L_{il}(T_0)r_i}{C_pT}\right]\right\}, \quad (27)$$

where we have taken L_{il}, L_{lv} and L_{iv} to be constant and evaluated at $T_0 = 273.16$ K. From (18) and (19) we know θ_{il} and θ_{eiv} are conservative (aside from the ϵ_1, ϵ_2, ϵ_3 and ϵ_4 errors mentioned above) for phase changes of water, but they become nonconservative in the presence of precipitation fluxes. The diagnosis of θ from the θ_L equivalent of (26) in a nonprecipitating system was shown by Wilhelmson (1977) to have a large positive bias at low temperatures which is attributable directly to the ϵ_1 error of inverse temperature.

In this study, we are concerned with finding a suitable alternative to the approximation in (26). Similar to Betts (1973), we employ a Taylor's series approximation to (26) given by

$$\theta_{il} = \theta\left[1 - \frac{L_{lv}(T_0)r_l}{C_pT} - \frac{L_{iv}(T_0)r_i}{C_pT}\right]. \quad (28)$$

Wilhelmson (1977) also showed that the θ_L equivalent to (28) resulted in similar errors to the θ_L equivalent of (26) when compared against a reversible, moist adiabat in a nonprecipitating system. This form also is identical to Deardorff's (1976) definition of θ_i. Eq. (26) also can be expanded in the inverse fashion giving

$$\theta = \theta_{il}\left[1 + \frac{L_{lv}(T_0)r_l}{C_pT} + \frac{L_{iv}(T_0)r_i}{C_pT}\right]. \quad (29)$$

Betts (personal communication) pointed out such a relationship will lead to slightly better evaluation of θ at midlevels, but must also lead to increasing error at low temperatures.

To compensate for these errors, we have introduced an empirical approximation to (29) which improves the accuracy in diagnosing θ. Because ϵ_1 grows very large at low temperatures, the accuracy in diagnosing θ can be improved by holding the temperature constant when it falls below 253 K. Thus the following empirical form of (29) is proposed:

$$\theta = \theta_{il}\left[1 + \frac{L_{lv}(T_0)r_l}{C_p \max(T, 253)}\right.$$
$$\left. + \frac{L_{iv}(T_0)r_i}{C_p \max(T, 253)}\right]. \quad (30)$$

Because θ_{il} and θ_{eiv} are conservative only in non-precipitating systems, changes of these quantities due to precipitation fallout must be considered in their practical application. This may be done in two ways. The first way is to consider that the total change in θ_{il} is given by

$$d\theta_{il} = d_i\theta_{il} + d_e\theta_{il}. \quad (31)$$

Applying (18), Eq. (31) becomes

$$d\theta_{il} = d_e\theta_{il}. \quad (32)$$

For the case of (30), we can differentiate and obtain

$$d\theta_{il} = d_e\theta_{il} = -\frac{\theta_{il}^2}{\theta}\frac{L_{lv}d_er_l + L_{iv}d_er_i}{C_p \max(T, 253)}, \quad (33)$$

where θ, L_{lv}, L_{iv}, C_p and T are intensive properties and therefore yield no external derivative. The external derivatives of r_l and r_i are the changes in those quantities due to precipitation. Similar expressions can be obtained also for (26)–(29).

Variations in θ_{il} and θ_{eiv} due to precipitation also are handled conveniently as an adjustment process. In the case of (30), we first compute all internal changes in r_l and r_v due to phase changes and diagnose the resulting θ, holding θ_{il} constant. Then, some fraction of r_l and r_i are removed to account for precipitation. Holding θ constant, (30) is then used to calculate a new θ_{il}. As a result, θ_{il} is conserved only as long as precipitation flux is not considered. From (1), we know external changes of r_l and r_i do not affect θ, and hence the isothermal adjustment to θ_{il} must also be valid. This adjustment method was applied to (26)–(30) and used in this study.

It will be shown experimentally in the next section that diagnosis of θ using (30) is very close to values diagnosed with (14) for both nonprecipitating systems and systems where precipitation is treated as an adjustment process. In a sense, it can be said that the maximum function introduces an error which corrects for the neglect of ϵ_1 and ϵ_2 in (20).

3. Tests of θ_{il} approximation in a simple one-dimensional Lagrangian model

In order to test the abovementioned forms of the first law of thermodynamics, a simple Lagrangian parcel model was constructed. The diagnosis of θ by (15) and (26)–(30) are compared to that made by (14) over two test situations. In the first test, a non-precipitating or closed system was considered for which θ_{il} and θ_{eiv} are conserved. In that test, although precipitation was allowed to form, its terminal velocity was set to be zero forcing it to move with the air parcel.

The results obtained from test 1 will tend to overestimate errors which should be expected when applying these approximations to precipitating systems, due to the high liquid water contents carried aloft. Therefore a second test was performed which

allowed precipitation to settle in a physically realistic manner. This test demonstrates the extent to which the loss of condensate improves the diagnosis of θ using the θ_{il} approximations in upper levels.

A third test also was performed which required all condensate to precipitate out as it was formed. This is equivalent to a pseudoadiabatic process. Because the ϵ_1 and ϵ_2 errors vanish as r_l and r_i go to zero, the θ variations diagnosed by (26) and (28)–(30) should be nearly indistinguishable from those obtained by (15) for the pseudoadiabatic process.

The model was run for both saturated ascent of a parcel containing liquid and ice water and unsaturated descent of an air parcel containing liquid water. For saturated ascent, an initially water-saturated parcel was assumed to have zero liquid and ice water contents. An initial potential temperature of 300 K was taken while the initial pressure was varied from one experiment to the next. The model was assigned an updraft velocity profile given by

$$ w = w_{\max} \left\{ \sin \left[- \frac{\pi(p - 100 \text{ kPa})}{100 \text{ kPa}} \right] \right\} , \quad (34) $$

where $w_{\max} = 10 \text{ m s}^{-1}$. This w profile is used strictly as a means to estimate a time scale associated with a given pressure change for use in the cloud microphysical calculations. Assuming the above initial conditions, pressure was lowered by 1 kPa increments leading to a temperature decrease within the parcel. From the hypsometric equation, the height scale associated with this pressure drop is given by

$$ \Delta Z = - \frac{RT}{g} \ln \left(\frac{p - 1 \text{ kPa}}{p} \right) , \quad (35) $$

where ΔZ is the height change, g is the acceleration of gravity and p is the pressure. Given the vertical updraft velocity w, the time taken for this ascent is

$$ \Delta t = \frac{\Delta Z}{w} . \quad (36) $$

Cloud water was diagnosed from the relation

$$ r_c = (r - r_{sv} - r_r - r_i) H(r - r_{sv} - r_r - r_i), \quad (37) $$

where H is the heaviside stepfunction given by

$$ H(x) = \begin{cases} 0, & x \leq 0 \\ 1, & x > 0. \end{cases} \quad (38) $$

The total liquid water is thus

$$ r_l = r_c + r_r. \quad (39) $$

The growth of rainwater mixing ratio by the processes of autoconversion and accretion of cloudwater was parameterized using the scheme described by Tripoli and Cotton (1980). The parameterization used to describe the rate of production of total ice water (r_i) at temperatures warmer than 233 K is de-

scribed by Stephens.[2] Cloud water colder than 233 K is set to zero and ice is assumed to grow by the ice adiabatic rate given by

$$ \frac{d_i r_i}{dt} \bigg)_{\text{moist}} $$
$$ = - \left(\frac{g w r_{si}}{RT} \right) \left[\left(\frac{\epsilon L_{iv}}{C_p T} - 1 \right) \bigg/ \left(\frac{\epsilon L_{iv}^2 r_{si}}{R C_p T^2} + 1 \right) \right] , \quad (40) $$

where $\epsilon = 0.611$. The ice and liquid water saturation mixing ratios (r_{si} and r_{sv}) were determined from the linearized form of the Goff Gratch equation described by Derickson and Cotton.[3] Mean terminal velocities of the assumed r_r and r_i distributions were determined by the rain and ice parameterizations. The greater time of residence experienced by rain and ice at the various pressure levels was accounted for by assuming rain and ice time scales given by

$$ \Delta t_r = \Delta t \frac{w}{w + V_r} , \quad (41) $$

$$ \Delta t_i = \Delta t \frac{w}{w + V_i} , \quad (42) $$

where V_r is the mean terminal velocity of rainwater and V_i is the mean terminal velocity of ice. These time scales were then used in conjunction with the growth rates of rain and ice in the test 2 case. In the closed system integrations (test 1), terminal velocities were set to zero; hence $\Delta t_r = \Delta t_i = \Delta t$.

Because growth rates and saturation mixing ratios are dependent upon temperature, an iteration was performed among the given form of the first law, the microphysical parameterizations, and (37)–(39) in order to evaluate a unique θ, T, r_c, r_r and r_i set. The iteration procedure is initiated with a first guess on θ and T assuming r_c is zero and r_r and r_i are specified from the parameterizations. Then r_{vs} is calculated leading to a possible new value for r_c. Next θ is reevaluated and 30% of the difference between the previous θ and the new evaluation is added to the previous θ for the next guess. This provides the next guess on T, r_{vs} and r_c. The iteration is complete when the reevaluated θ has converged to within 0.001 K of the previous θ estimate.

Integrated forms given by

$$ \theta_2 = \theta_1 \exp \left[\left(\frac{\bar{R}_m}{\bar{C}_{pm}} - \frac{R}{C_p} \right) \ln \left(\frac{P_2}{P_1} \right) \right. $$
$$ \left. + \frac{L_{lv}(\bar{T})}{\bar{C}_{pm} \bar{T}} (r_{v2} - r_{v1}) + \frac{L_{il}(\bar{T})}{\bar{C}_{pm} \bar{T}} (r_{i2} - r_{i1}) \right] \quad (43) $$

[2] Stephens, M. A., 1979: A simple ice phase parameterization. Atmos. Sci. Pap. No. 319, Colorado State University, NSF Grant ATM77-09770, 122 pp.

[3] Derickson, R. G., and W. R. Cotton, 1977: On the use of finite Taylor series approximations to certain exponential and power functions employed in cloud models. Atmos. Sci. Pap. No. 268, Colorado State University, NSF Grant DES 7513310, 19 pp.

for (14) and

$$\theta_2 = \theta_1 \exp\left[- \frac{L_{lv}(\bar{T})}{C_p \bar{T}} (r_{v2} - r_{v1}) \right.$$

$$\left. + \frac{L_{il}(\bar{T})}{C_p \bar{T}} (r_{i2} - r_{i1}) \right] \quad (44)$$

for (15) were used to determine the new θ. The subscripts 1 and 2 refer to the previous and predicted values respectively, while the overbars represent the average of the position 1 and position 2 values. It should be noted that these predictions do not include external changes in r_i due to precipitation fallout. These changes are made (for the test 2 and test 3 calculations) as an isothermal and isobaric adjustment process which is described below. In the cases of (26)–(30), no finite differencing is necessary to determine θ.

In the open system (tests 2 and 3) calculations, precipitation adjustments to rain and ice were made isothermally and isobarically after the closed system calculations described above were complete. In the test 2 case, assuming the vertical variations in rainwater and ice water are such that their mixing ratios decrease to zero 10 pressure increments above the parcel pressure level, a forward-upstream time and space operator was employed to determine the losses to rain and ice. This operator is given by

$$\Delta r_r = \frac{V_r r_r}{10} \frac{\Delta t}{\Delta Z} \quad (45)$$

for rain, and

$$\Delta r_i = \frac{V_i r_i}{10} \frac{\Delta t}{\Delta Z} \quad (46)$$

for ice losses. For test 3, in which all condensate was removed, changes in rain, cloud water and ice were given simply by

$$\Delta r_r = -r_r, \quad (47)$$

$$\Delta r_c = -r_c, \quad (48)$$

$$\Delta r_i = -r_i. \quad (49)$$

The values of θ_{il} or θ_{eiv} were then recalculated holding p and θ constant.

Calculations were also performed for both test 1 and test 2 for the case of unsaturated descent of an initially water-saturated air parcel containing 6.0 g kg^{-1} rainwater and 0.0 g kg^{-1} cloudwater at a given pressure value. In this case, the evaporation of rain was the only physical process considered. The parameterization of rain evaporation is described by Tripoli and Cotton (1980).

These simple model calculations led to a change in θ with decreasing pressure characteristic of each form of the first law tested. The computed characteristic potential temperature lapse rates were then compared to that given by (14) in order to evaluate the relative accuracy of the approximation.
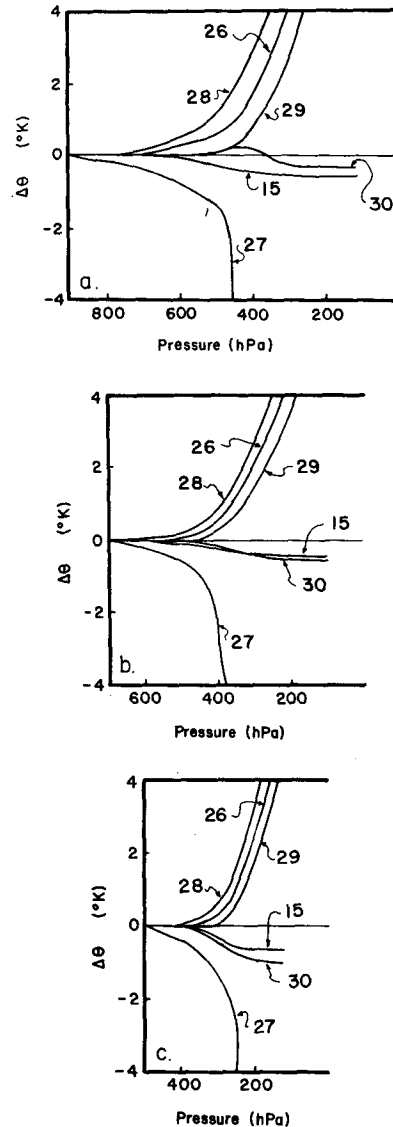

Fig. 1. Test 1 (zero precipitation fall velocity) differences between θ diagnosed by (14) and the equations labeled as a function of pressure for a rising parcel. Calculations are performed for a parcel initially liquid water saturated at (a) 90 kPa, (b) 70 kPa and (c) 50 kPa pressure rising to 11 kPa. Initial potential temperature was 300 K in each case.

4. Results

For tests 1, 2 and 3, vertical variations of potential temperature were computed using (15) and (26)–(30), and then compared to the results using (14). Fig. 1 shows the calculated differences between the various schemes starting from different base pressures for moist ascent for test 1. Variations similar to those shown by Wilhelmson (1977) are noted for θ_{il} using the expressions similar to those he tested, although superior performance has been obtained at higher temperatures perhaps from the iterative treatment on θ based on more exact formulations of saturation over water and ice. The differences ob-

TABLE 1. Root-mean-square error (K) accumulated by each diagnostic technique in evaluating θ starting from initial pressure value and ending at final pressure value. Tests 1 and 2 refer to tests with non-precipitating and precipitating systems.

Initial pressure– final pressure (kPa)	Eq. (15)		Eq. (26)		Eq. (27)		Eq. (28)		Eq. (29)		Eq. (30)	
	Test 1	Test 2	Test 1	Test 2	Test 1	Test 2	Test 1	Test 2	Test 1	Test 2	Test 1	Test 2
90–11	0.40	0.31	4.66	3.32	6.23	5.16	5.99	4.19	3.55	2.56	0.19	0.13
70–11	0.29	0.20	3.10	2.80	4.19	4.09	3.67	3.30	2.58	2.34	0.31	0.23
50–11	0.41	0.17	2.37	2.41	3.94	4.13	2.87	2.87	1.92	1.97	0.63	0.41
50–94	0.13	0.07	0.46	0.36	1.90	0.74	0.79	0.64	0.15	0.10	0.15	0.10
70–94	0.08	0.05	0.31	0.21	0.62	0.27	0.45	0.33	0.18	0.09	0.18	0.09

tained by (26), (28) and (29) are again exponential as were those of Wilhelmson (1977) because of the inverse temperature effect described previously when ice or liquid water is present at low temperatures. The curve for (30) shows this error was eliminated by using the given empirical relationship; the

FIG. 2. As in Fig. 1 except for test 2 (nonzero precipitation fallspeed).

results are comparable to (15). It was not attempted, but empirical adjustments can probably be made of θ_{eiv} to increase its accuracy as was done with θ_{il}. The root-mean-square (rms) errors are given for each scheme in Table 1.

Fig. 2 shows the temperature variations produced by test 2 when precipitation was allowed to settle in a physically realistic manner from the developing updraft. We note a slightly improved performance by θ_{il} formulations due to the reduced magnitude of ϵ_1 and ϵ_2 which are weighted by liquid and ice condensate.

The results obtained for test 3, where all condensate was required to precipitate out instantaneously, demonstrated (as expected) that the variation in θ diagnosed by (26) and (28)–(30) were nearly indistinguishable from those diagnosed by (15). The rms errors in the θ diagnosed by (15) was only about one-quarter of those produced by test 1 because of the lower amounts of total water carried aloft. This minimizes the error associated with neglecting heat storage by water. As a result, errors in diagnosing θ from (27) were also reduced in test 3. Because the errors were so small in test 3, profiles of θ would be indistinguishable from the abscissa in graphs like Fig. 1. Therefore, the results of test 3 were not plotted.

The downdraft cases for test 1 and test 2 are shown in Figs. 3 and 4. It can be seen that much better results are obtained in all the pseudo-adiabatic approximations as a consequence of the reduced inverse temperature error effects. Again, (30) produces results nearly as good or better than (15) in both the open and closed system cases. In calculations not reported here, it was found (15) and (30) result in somewhat greater error at upper levels when ice is not present. This is also demonstrated by Wilhelmson (1977) and Lipps and Hemler (1980) for the case of (15). These results clearly demonstrate a sufficiently accurate diagnosis of θ by (30) to allow θ_{il} to be considered as a thermodynamic variable conservative over all water phase changes in deep convective processes.

5. Discussion and conclusions

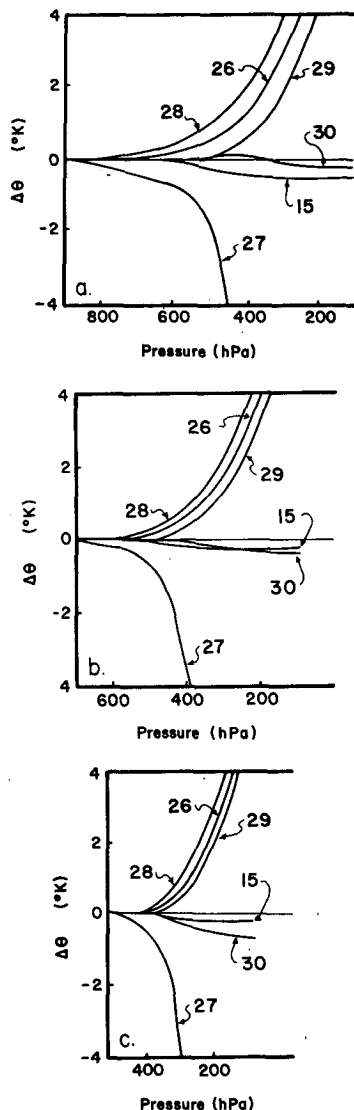The use of ice-liquid water potential temperature along with total water has been determined a viable

and powerful alternative to the use of potential temperature, water vapor and cloud water as time-dependent prognostic variables in moist, deep atmospheric models. Simple Lagrangian, parcel model calculations, encompassing the effects of fallout of rain and ice, have clearly demonstrated the accuracy of this system for reversible and irreversible processes.

The incorporation of θ_{il} into a cloud model eliminates the need for saturation adjustment procedures. Such procedures require numerous approximations and sudden adjustments which can lead to numerical "shocks" or computational noise. The incorporation of θ_{il} also reduces the number of time-dependent variables by one. This occurs as water vapor is replaced by total water and cloud water becomes diagnostic. As temperatures become very cold, cloud ice may be diagnosed instead of cloud water, if the ice phase is considered. Water phase changes between liquid, ice and vapor are greatly simplified in this system since tendencies on temperature do not need to be considered. The only source term on θ_{il} which must be considered is that due to movement of ice or liquid water relative to the air by precipitation. This is simply accomplished by taking the differen-
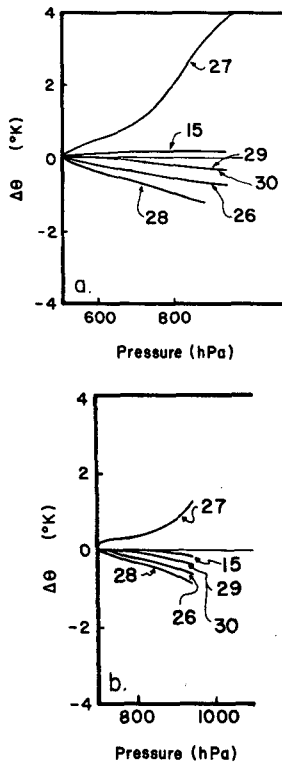

FIG. 4. As in Fig. 3 except for test 2 (nonzero precipitation fallspeed).

FIG. 3. Test 1 (zero precipitation fallspeed) differences between θ diagnosed by (14) and the equations labeled as a function of pressure for a sinking parcel. Calculations are performed for a parcel with no ice which initially contains 6 g kg^{-1} of rainwater at (a) 50 kPa, and (b) 70 kPa sinking to point at which all water is evaporated.
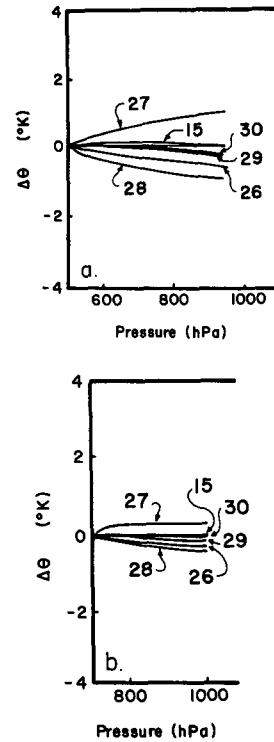
tial (33) with respect to time. The resulting relationship is given by

$$\frac{d\theta_{il}}{dt} = - \frac{\theta_{il}^2}{\theta}$$

$$\times \left[\frac{L_{lv}\left(\dfrac{dr_l}{dt}\right)_{\text{precip}} + L_{iv}\left(\dfrac{dr_i}{dt}\right)_{\text{precip}}}{C_p \max(T, 253)} \right]. \quad (50)$$

Because a time tendency on pressure is difficult to formulate simply in the θ_{il} system, density may be used as the predictive quantity instead. In the case of an anelastic model, the θ_{il} system would not affect the pressure diagnostic equation.

The thermodynamic variable θ_{il} has already been incorporated into the CSU multi-dimensional cloud/mesoscale model. The iteration procedure increases the time required to perform a single time step integration by over a factor of 2 at grid points where cloud water is present. However, since it is only a small fraction of all grid points containing condensate, overall timing increases <10%. It is our belief that the added simplicity without loss of accuracy which we obtain from this thermodynamic system far outweighs the disadvantage of added computer cost when modeling deep tropospheric convection. Moreover, use of such a thermodynamic variable also greatly simplifies the formulation of a cloud or mesoscale model using higher order turbulence closure techniques.

APPENDIX

List of Symbols

A_{il}	affinity of melting (J kg^{-1})
A_{lv}	affinity of vaporization (J kg^{-1})
C_i	specific heat of ice water [$=2.1 \times 10^3$ J K^{-1} kg^{-1}]
C_l	specific heat of liquid water [$=4.187 \times 10^3$ J K^{-1} kg^{-1}]
C_p	specific heat of dry air at constant pressure [$=1.003 \times 10^3$ J K^{-1} kg^{-1}]
C_{pm}	specific heat of moist air at constant pressure (J K^{-1} kg^{-1})
C_{vp}	specific heat of water vapor at constant pressure [$=1.846 \times 10^3$ J K^{-1} kg^{-1}]
e_{si}	saturation vapor pressure with respect to ice water (kPa)
e_{sv}	saturation vapor pressure with respect to liquid water (kPa)
e_v	water vapor pressure (kPa)
g	acceleration of gravity (m s^{-2})
H	heaviside step function
L_{iv}	latent heat of sublimation (J kg^{-1})
L_{il}	latent heat of melting (J kg^{-1})
L_{lv}	latent heat of vaporization (J kg^{-1})
p	total pressure of air (kPa)
p_d	pressure of dry air (kPa)
R	dry air gas constant [$=0.287 \times 10^3$ J K^{-1} kg^{-1}]
R_v	water vapor gas constant [$=0.462 \times 10^3$ J K^{-1} kg^{-1}]
R_m	moist air gas constant (J K^{-1} kg^{-1})
r	mixing ratio of total water
r_c	mixing ratio of cloud water
r_i	mixing ratio of ice water
r_l	mixing ratio of liquid water
r_r	mixing ratio of rain water
r_{si}	saturation mixing ratio with respect to ice water
r_{sv}	saturation mixing ratio with respect to liquid water
r_v	mixing ratio of vapor water
t	time scale for air parcel (s)
t_r	time scale for rainwater (s)
t_i	time scale for icewater (s)
T	temperature (K)
T_0	273 K
V_i	average terminal velocity of ice (m s^{-1})
V_r	average terminal velocity of rain (m s^{-1})
w	vertical velocity of air parcel (m s^{-1})
w_{max}	amplitude of sine function giving w profile (m s^{-1})
Z	height above ground (m)
ϵ	ratio of molecular weight of moist air to that of dry air [$=0.611$]
ϵ_1	error involved in θ_{il} approximation associated with r_l term
ϵ_2	error involved in θ_{il} approximation associated with r_i term
ϵ_3	error involved in θ_{eiv} approximation associated with r_v term
ϵ_4	error involved in θ_{eiv} approximation associated with r_i term
μ_0	base state chemical potential (J kg^{-1})
μ_i	chemical potential of interface of a plane surface of ice water and air (J kg^{-1})
μ_v	chemical potential of water vapor (J kg^{-1})
μ_l	chemical potential of interface of a plane surface of liquid water and air (J kg^{-1})
θ	potential temperature of air (K)
θ_{eiv}	equivalent ice vapor potential temperature (K)
θ_i	Deardorff's equivalent to θ_{il} (K)
θ_{il}	ice-liquid water potential temperature (K).

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