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Wet Equivalent Potential Temperature and Enthalpy as Prognostic Variables in Cloud Modeling

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ABSTRACT

The bulk thermodynamic consequences of nonreversible phase changes and of the precipitation process are emphasized. Two predictive quantities are proposed, either of which can be used as a prognostic thermodynamic variable, instead of temperature or of potential temperature, in numerical models of convective clouds. The use of these new variables decreases the coupling between the dynamical and the thermodynamical equations and is shown to induce smaller errors under most circumstances involving physical processes such as the freezing of supercooled drops and the evaporation in undersaturated air. The respective advantages of both variables are discussed; the choice between them is shown to depend upon the phenomena to be simulated.

1. Introduction

The numerical simulation of the flows which develop in a deep cumulonimbus cloud involves the solution of equations appropriate to a multiphase mixture of compressible gases, liquids and solids in which phase changes (condensation, evaporation, sublimation, freezing) take place. These equations must be able to describe as accurately as possible such aspects as the nonreversible phase changes (freezing of supercooled drops, evaporation in subsaturated air), the spatial transport of liquid water due to precipitation, and the nonhydrostatic part of the pressure which are some of the essential features of such flows. Therefore, the bulk thermodynamics of these phenomena should be accurately treated in a simple manner. However, the fundamental thermodynamical equation, obtained by applying an enthalpy conservation principle to a non-equilibrium open system, involves the rate of change of the partial pressure, the mixing ratio and the temperature of each phase, and is not very easy to integrate.

Although considerable attention has been paid to the thermodynamic equations (Betts, 1973; Iribarne and Godson, 1973; Dutton, 1976; Wilhelmson, 1977; Brook, 1978; Simpson, 1978; Paluch, 1979; Bolton, 1980; Tag, 1980; Lipps and Hemler, 1980) and to the equations appropriate to multiphase flows (Das, 1969; Tripoli and Cotton, 1981), it seems that all the terms which appear in the fundamental bulk thermodynamical equation have not yet been completely accounted for. The first goal of the present paper is to provide a complete formulation of the bulk thermodynamics of a convective cloud as well as to emphasize the thermodynamics of nonreversible phase changes.

In addition, two thermodynamical quantities are

proposed for use as prognostic variables in numerical models instead of the mean temperature or one of the previously proposed potential temperatures (Betts, 1973; Wilhelmson, 1977; Paluch, 1979; Tripoli and Cotton, 1981). For cloud modeling, it is essential to make the right choice for this quantity since, as shown by several authors (Madden and Robitaille, 1970; Betts, 1973; Simpson, 1978), the maximum altitude of cumulus cloud predicted with the use of a thermodynamic equation is strongly dependent upon the conservative quantity used for the prediction. It is true that in three-dimensional cloud modeling, other factors such as the subgrid parameterization scheme (turbulence closure), the dynamical scheme (hydrostatic versus nonhydrostatic, fully compressible versus anelastic), the boundary conditions and the initial conditions may be even more important. However, the bulk thermodynamical aspect of the flow is probably the first to consider when trying to avoid approximations made in earlier studies. These approximations are becoming more and more unnecessary due to the improvements in computers and in numerical methods of integration.

In Section 2, the basic equations are derived and justifications are provided for some approximations; in Section 3, numerical computations are performed in order to examine, in some extreme cases, the validity of the proposed "conservative" thermodynamical quantities. Analyses of the simulation results are given in Section 4.

2. Formulation

The cloudy air consists of dry air (index d), of water vapor (index v), of liquid water (index l) and of ice particles (index i). In this work, water vapor and dry

air are treated as perfect gases with constant specific heats. Although molecular diffusion is important in estimating the rate of change of each drop radius, its effects on a characteristic length scale greater than a few decimeters are much less than the effects of turbulent diffusion which is not considered here. The mixing ratios and all the species' properties are defined as mean values over a volume which is of the order of a few cubic decimeters, i.e., large enough so that a large number of particles are in this volume, but small enough so that it can be considered homogeneous. The water vapor does not have homogeneous properties throughout the averaging volume considered since its temperature and mixing ratio vary around each drop due to the diffusive processes of heat and vapor. However, in general, the relative mass of water vapor directly affected by the drops is small and, therefore, the mean value of the water vapor temperature is taken as that of the dry air. The partial pressure of water vapor is generally below the saturated value at the corresponding temperature; condensation occurs as soon as this value is exceeded. The volume of the liquid water is neglected, compared to the specific volume of the water vapor (the error is less than 0.002), but the energy carried by the water or ice particles is fully considered.

The liquid water is assumed to consist of droplets which have a relative velocity \mathbf{V}_l in the air, a mean temperature T_l and a concentration ρ_l (kg m^{-3}) or a mixing ratio $r_l = \rho_l/\rho_d$ (kg kg^{-1}). The difference between the air temperature T and the droplet temperature T_l can be of the order of several degrees (Pruppacher and Klett, 1978) for drops of radius greater than 1 mm falling in subsaturated air. The time evolution of the drop temperature can be obtained from the heat budget of each drop; the adaptation time of the drop temperature to its steady-state value can be as large as 4.4 s for a drop of radius 1.35 mm. Therefore, in the averaging volume, all drops of the same radius are assumed to have the same origin and identical properties which can be different from those of other drops. For simplicity, in the following derivation, all drops are assumed to have the same radius; this gives no loss of generality since generalization of the following equations to many classes of drops having different radius, temperatures and terminal velocities is straightforward and will be done in Section 3.

The solid phase is assumed to have a concentration ρ_s , a mixing ratio $r_s = \rho_s/\rho_d$ (kg kg^{-1}), a temperature T_s and a mean relative velocity \mathbf{V}_s . Similar to the case of liquid particles, the generalization to many classes of ice particles is straightforward.

a. The basic thermodynamic equation

Dutton (1976) has considered the enthalpy variation during any change appearing in an open system and developed the first law of thermodynamics for such a case [see Tripoli and Cotton, 1981; their Eq. (1)]. Dut-

ton's equation is written in terms of internal and external derivatives ($d_i\chi/dt$ and $d_e\chi/dt$, respectively). The former derivative describes the change along the parcel path; the latter results from the energy flux into or out of the parcel and is here considered to be associated with the derivative along the relative motion of the precipitating particles alone. For example, and for any quantity χ (a list of symbols is given in the Appendix), we have

$$\frac{d_e}{dt}(r_l\chi) = \mathbf{V}_l \cdot \nabla(r_l\chi),$$

or

$$r_l \frac{d_e}{dt}(\chi) = r_l \mathbf{V}_l \cdot \nabla(\chi),$$

while

$$\frac{d_e}{dt}(r_v\chi) = \frac{d_e}{dt}(s_d) = 0.$$

With this interpretation of Dutton's notation, the fundamental thermodynamical equation used in this paper reads, with the usual notations,

$$\begin{aligned} & \frac{d}{dt}(C_{pd} \ln T) - \frac{d}{dt}(R_d \ln P_d) + \frac{d}{dt}\left(r_v \frac{L_{lv}}{T}\right) \\ & - \frac{d}{dt}\left(r_l \frac{L_{il}}{T}\right) + r_v \frac{d}{dt}\left(\frac{A_{lv}}{T}\right) - r_l \frac{d}{dt}\left(\frac{A_{il}}{T}\right) \\ & + r_T C_l \frac{d}{dt} \ln T + r_l C_l \mathbf{V}_l \cdot \nabla \ln T_l \\ & - r_l \mathbf{V}_l \cdot \left[\nabla \left(\frac{A_{il}}{T} \right) - C_l \nabla \ln T_l \right] = 0, \quad (1) \end{aligned}$$

where d/dt is the time derivative following the air and water vapor (internal derivative in Dutton's notation), i.e.,

$$d/dt = \partial/\partial t + \mathbf{u} \cdot \nabla, \quad (2)$$

where \mathbf{u} is the air (and water vapor) velocity.

The term $r_T C_l d/dt \ln T$ in (1) represents energy change due to a water mass being advected with the fluid medium (Orville and Kopp, 1977). The term $r_l C_l \mathbf{V}_l \cdot \nabla \ln T_l$ has already been obtained by Das (1969) and represents the cooling effect due to the downward flux, through the air parcel, of precipitating particles which warm up under a forced conduction process at the expense of the air parcel energy. The last term in (1) is partly due to the energy caught away by the precipitating ice particles and partly due to nonreversible change of entropy associated with the freezing process.

The affinity term A_{lv} (A_{il}) is defined as the change in the free enthalpy of water going from the liquid to the vapor state (from the ice to the liquid state) such that

$$A_{lv} = h_l - T_l s_l - h_v + T_v s_v \simeq \bar{T}(s_v - s_l) - L_{lv}, \quad (3)$$

$$A_{il} = h_i - T_i s_i - h_l + T_l s_l \simeq \bar{T}_i(s_l - s_i) - L_{il}, \quad (4)$$

where \bar{T} (\bar{T}_i) is a mean temperature between T and T_l (T_l and T_i). The last equalities hold because the phase changes occur at a constant total pressure (Dutton, 1976) and because the temperatures T_l , T_v , T_i are not very different. These last equalities will be used to evaluate the affinity terms.

The affinity due to nonreversible processes can be assumed to be of the order of magnitude of the corresponding free enthalpy difference experienced along a reversible process going from the same initial state to the final one. Two different processes can be considered which start from liquid water at the temperature T_l and lead to water vapor at the temperature T and at the pressure e_v (partial pressure of water vapor in the dry air). The first one evaporates the water at the temperature T_l , giving water vapor with the partial pressure $e_s(T_l)$ and then heats (or cools) the water vapor to the temperature T while expanding it to the partial pressure e_v . The entropy change is therefore

$$(s_v - s_l)_1 = L_{lv}(T_l)/T_l + C_{pv} \ln(T/T_l) - R_v \ln[e_v/e_s(T_l)]. \quad (5)$$

The second process warms (or cools) the liquid water to the temperature T , evaporates the water at this temperature, and expands the water vapor from the pressure $e_s(T)$ to the pressure e_v . The corresponding entropy change is

$$(s_v - s_l)_2 = \frac{L_{lv}(T)}{T} - C_l \ln(T/T_l) - R_v \ln[e_v/e_s(T)]. \quad (6)$$

The use of the Clausius-Clapeyron's relation

$$\frac{de_s(T)}{dT} = \frac{L_{lv}(T)e_s(T)}{R_v T^2}, \quad (7)$$

together with Kirchhoff's law

$$\frac{dL_{lv}}{dT} = C_{pv} - C_l, \quad (8)$$

shows that these two functions of T and T_l as given by (5) and (6) are identical. This enables the evaluation of the affinity A_{lv} by inserting (6) in (3), giving

$$A_{lv} \approx -R_v T \ln[e_v/e_s(T)], \quad (9)$$

where the second term in (6), which is an order of magnitude smaller than the third one, has been neglected and where the mean temperature \bar{T} has been approximated by the air temperature T . This affinity term can be of the order of several percent of the latent heat of vaporization and should not be neglected in the simulation of flows in which drops evaporate in subsaturated air.

Similarly, the nonreversible process which consists in the freezing of supercooled droplets (at a temperature T_i which can be as low as -20 to -40°C) gives an entropy change which can be assumed to be of the

order of the change produced by the following hypothetical reversible process. In this latter process, the supercooled water is warmed up to the temperature $T_0 = 273.1$ K; freezing occurs and the ice is cooled back to the temperature T_i .

$$s_l - s_i = C_l \ln(T_l/T_0) + L_{il}(T_0)/T_0 + C_i \ln(T_0/T_i). \quad (10)$$

In the case of freezing, the drop temperature T_l cannot depart very much from the air temperature T and, likewise, since the latent heat of freezing is small, the ice temperature T_i is also close to the air temperature T . This affinity can be approximated by

$$A_{il} \approx T \left[\frac{L_{il}(T_0)}{T_0} - \frac{L_{il}(T)}{T} + (C_l - C_i) \ln\left(\frac{T}{T_0}\right) \right], \quad (11)$$

which is a function of the temperature T alone. This affinity term can reach 20% of the latent heat of freezing and is identical to the expression proposed by Tripoli and Cotton (1981):

$$A_{il} = R_v T \ln[e_i(T)/e_s(T)],$$

if the saturated vapor pressure over ice is related to the latent heat of sublimation by the Clausius-Clapeyron equation.

Equation (1), in which the affinity terms are evaluated from (9) and (11), is the fundamental thermodynamical equation used in this study. It relates the rate of change of temperature to those of the partial pressures and the mixing ratios under any circumstances (nonreversible phase changes, precipitation processes); equilibrium is not assumed. It differs from Tripoli and Cotton's (1981) fundamental equation [their Eq. (14)], by explicitly showing the influence of the precipitating particles [last terms in (1)] instead of using the internal and external derivatives. Eq. (1) shall be used as a norm to which the approximate equations will be compared.

In fact, Eq. (1) is not of practical use in numerical models since it is strongly coupled to the pressure tendency equation and to the microphysical equations predicting the value of the mixing ratios. It is, therefore, essential to define a quantity which has a much smaller variation along the particle path and is less dependent upon the fluctuations of partial pressures and of mixing ratios than the temperature. Two such quantities are defined in the next two subsections.

Tripoli and Cotton (1981) have already considered several approximations and proposed an ice-liquid potential temperature (ILPT) defined by

$$\theta \left[1 + \frac{L_{lv}(T_0)(r_i + r_l) + L_{il}(T_0)r_l}{C_{pd} \max(T, 253.)} \right]^{-1}, \quad (12)$$

where the potential temperature θ is given by Poisson's equation

$$\theta = T(P_0/P)^{R_d/C_{pd}}, \quad (13)$$

and $P_0 = 1000$ mb. It will be shown in the third part of this paper that, in some extreme situations, this ice-liquid potential temperature leads to errors of up to 5 K in the evaluation of the potential temperature of a moist parcel and is not the most accurate quantity to be considered.

b. Wet equivalent potential temperature (WEPT)

In order to derive a new potential temperature, two approximations can be considered.

- The first approximation involves the replacement of the term

$$r_v \frac{d}{dt} \left(\frac{A_{lv}}{T} \right) \text{ by } \frac{d}{dt} \left(r_v \frac{A_{lv}}{T} \right).$$

This replacement induces no errors in two cases:

- 1) When $A_{lv} \approx 0$; this occurs during the condensation since the supersaturation is very small in clouds and $e_v \approx e_s(T)$.
- 2) When r_v is constant; this occurs when the moist air does not contain liquid or ice particles.

- Similarly, the second approximation replaces

$$r_i \frac{d}{dt} \left(\frac{A_{il}}{T} \right) \text{ by } \frac{d}{dt} \left(r_i \frac{A_{il}}{T} \right).$$

The magnitude of the terms involved by these approximations is only a few percent of the magnitude of the dominant terms in (1).

With these two approximations, the thermodynamic equation is approximated by

$$C_{pt} \frac{d \ln T}{dt} - R_d \frac{d \ln P_d}{dt} + \frac{d}{dt} \{ [L_1(T)r_v - L'(T)r_i]/T \} + \left\{ r_i \mathbf{V}_i \left[C_l - \frac{L_{il}}{T} \right] + C_l r_l \mathbf{V}_l \right\} \cdot \nabla \ln T = 0, \quad (14)$$

where

$$\begin{aligned} C_{pt} &= C_{pd} + r_T C_l, \\ L_1(T) &= L_{lv}(T) - R_v T \ln [e_v/e_s(T)], \\ L(T) &= L_{il}(T) + A_{il}(T). \end{aligned}$$

One consequence of this equation is that the wet equivalent potential temperature (WEPT), defined by

$$\theta_q = T(P_0/P_d)^{R_d/C_{pt}} \exp\{ [L_1(T)r_v - L'(T)r_i]/(TC_{pt}) \}, \quad (15)$$

has a rate of change which follows the equation

$$C_{pt} \frac{d \ln \theta_q}{dt} = \ln(T/\theta_q) C_l \frac{dr_T}{dt} - \left[r_i \mathbf{V}_i \left(C_l - \frac{L_{il}}{T} \right) + C_l r_l \mathbf{V}_l \right] \cdot \nabla \ln T, \quad (16)$$

where the first term on the right-hand side results from the variation of C_{pt} within the exponent. The change in the total mixing ratio r_T is due to precipitations and is easily shown to be given by (Das, 1969)

$$\frac{dr_T}{dt} = \nabla \cdot (\rho_l \mathbf{V}_l + \rho_i \mathbf{V}_i) / \rho_d. \quad (17)$$

Therefore, the wet equivalent potential temperature θ_q is essentially constant (within the two approximations shown in Section 2b) during any transformation even when it involves phase changes, except when precipitating particles are present. Paluch (1979) has used a similar quantity (without the ice phase) in an experimental study of the entrainment in clouds; however, two different expressions were found to be necessary, corresponding to undersaturated and saturated conditions. Keeping the affinity of condensation A_{lv} in the thermodynamical equation makes it possible to define this unique expression [Eq. (15)].

As shown in Section 3, it is easy to set up an iterative scheme in order to compute the temperature T and the vapor mixing ratio from the values of the wet equivalent potential temperature. However, the main difficulty with its use in numerical models lies in the fact that its evaluation involves the lengthy computations of exponential, logarithmic and power functions.

c. Wet equivalent enthalpy (WEE)

A second approach to the simplification of the basic thermodynamical equation (1) is as follows.

On elimination of the partial pressure of dry air through the state equations, (1) can be exactly rewritten as

$$\begin{aligned} (C_{pd} + r_T C_l) \frac{dT}{dt} - \frac{(1 + r_T) dP}{\rho_T} + \frac{d}{dt} (L_{lv}(T)r_v) - T \frac{d}{dt} \left[\frac{L'(T)r_i}{T} \right] + A_{il} \frac{dr_i}{dt} + \left[r_i \mathbf{V}_i \left(C_l - \frac{L_{il}}{T} \right) + C_l r_l \mathbf{V}_l \right] \cdot \nabla T = 0, \quad (18) \end{aligned}$$

where $\rho_T = \rho_d(1 + r_T)$ is the total density. This equation can be further modified in order to eliminate the water vapor mixing ratio in favor of the total mixing ratio, i.e.,

$$r_v = r_T - r_l - r_i. \quad (19)$$

Some straightforward algebra leads to

$$\begin{aligned} C_{pd}(1 + \epsilon' r_T) \frac{dT}{dt} - \frac{(1 + r_T) dP}{\rho_T} - \frac{d}{dt} [L_{lv}(r_l + r_i)] - T \frac{d}{dt} \left[\frac{L'(T)r_i}{T} \right] + A_{il} \frac{dr_i}{dt} + L_{lv}(T) \frac{dr_T}{dt} + \left[r_i \mathbf{V}_i \left(C_l - \frac{L_{il}}{T} \right) + C_l r_l \mathbf{V}_l \right] \cdot \nabla T = 0, \quad (20) \end{aligned}$$

where $\epsilon' = C_{pv}/C_{pd}$ is the ratio of the specific heat at constant pressure of water vapor to that of dry air.

This energy equation shows that the wet equivalent enthalpy (WEE) defined by

$$H1 = C_{pd}[1 + (\epsilon' - 1)r_T]T - gz - \left[L_{iv}(T)(r_l + r_i) + T_0 \frac{L'(T)r_i}{T} \right] (1 - r_T) \quad (21)$$

is almost conserved under any adiabatic process involving nonreversible phase changes without precipitating particles. Indeed, the rate of change of the wet equivalent enthalpy is approximately given by

$$\begin{aligned} \frac{dH1}{dt} \approx & -[r_i \nabla_i (C_l - L_{il}/T) + C_l r_l \nabla_l] \cdot \nabla T (1 - r_T) \\ & + \frac{1}{\rho_T} \left[\frac{d}{dt} (P) - \rho_T g w \right] \\ & + \frac{dr_T}{dt} [C_{pd} T (\epsilon' - 1) - L_{iv} (1 - r_T - r_l - r_i)]. \quad (22) \end{aligned}$$

The first term on the right-hand side is due to the energy caught by the precipitating particles which come from higher altitudes with a lower temperature and fall through the moist air exchanging energy with the air parcel. The second term vanishes in hydrostatic atmospheres but should not be neglected inside deep convective clouds. The third term arises from the fact that the wet equivalent enthalpy is an extensive quantity which must vary when the total mixing ratio changes. The wet equivalent enthalpy is at most quadratic in the various parameters and, as shown in the third part, it is easy to set up an iterative scheme in order to solve for the parcel temperature knowing its enthalpy, its altitude, and the rain, ice, graupel and total mixing ratios.

3. Numerical evaluation of the errors using a Lagrangian model

Following Tripoli and Cotton (1981), numerical computations are carried out in order to estimate the errors involved in the simulation of convective flows using the two different approximations considered in this work. The basic equation considered in this paper, namely (1), in which the affinity terms are evaluated from (9) and (11), is solved for the temperature at the next level $[T(P + \Delta P)]$. This temperature is considered as the reference value to which the parcel temperatures, deduced from the potential temperatures or enthalpy, are compared. The differences between the corresponding potential temperatures indicate the errors that can be made when any of these quantities (potential temperatures or enthalpy) is used as a predictive quantity in a numerical model instead of using the complete basic equation.

Three tests have been conducted under the following general conditions. The parcel rises in a hydrostatic atmosphere with a vertical velocity which is a function of the total pressure alone given by

$$w(P) = w_{max} \sin[(P_1 - P)\pi/P_1], \quad (23)$$

where $w_{max} = 10 \text{ m s}^{-1}$ and $P_1 = 1100 \text{ mb}$.

The microphysical structure of the parcel is characterized by five mixing ratios of the different water species: r_v for the water vapor, r_c for the cloud droplets, r_r for the precipitating drops, r_i for the ice crystals and r_h for the precipitating graupel. The microphysical equations are similar to those used by Tripoli and Cotton and imply no supersaturation. Condensation/evaporation of cloud droplet (r_c) occurs whenever the partial pressure of water vapor becomes larger/smaller than its saturated value. The function $e_s(T)$ is obtained as the result of the analytical integration of the Clausius-Clapeyron equation [(7)] in which the latent heat of vaporization is a linear function of the temperature satisfying (8).

In each case, the parcel starts its ascent from 1000 mb where it has a temperature of 310 K and a total mixing ratio of 0.02. It rises up to 100 mb and then descends back to the 1000 mb level with the negative vertical velocity given by (23) with $w_{max} = -10 \text{ m s}^{-1}$. During the descent, the rain and graupel particles evaporate slowly according to the microphysical equations.

The integration scheme is based on the iterative solution of the implicit equation

$$\chi(P + \Delta P) = \chi(P) - \Delta P \frac{d\chi}{dt} (\bar{P}, \bar{T}, \bar{r}) / (\bar{\rho}_T g \bar{w}), \quad (24)$$

where χ stands for any parameter and where quantities with overbars are evaluated as mean values between the values at the upper and at the lower level. The pressure increment ΔP is adjusted so that the change in mixing ratios remains between 10^{-5} and 5×10^{-5} and the corresponding time step is less than 10 s.

In the discretization of the rate equations, the terms involving the time derivatives are all evaluated as

$$\begin{aligned} A(P, T, r) \frac{d\chi}{dt} \approx & \frac{1}{2} \left[\frac{\chi(P + \Delta P) - \chi(P)}{\Delta P} \right] [A(P + \Delta P, \\ & T + \Delta T, r + \Delta r) + A(P, T, r)] / (\bar{\rho}_T g \bar{w}), \quad (25) \end{aligned}$$

where $A(P, T, r)$ is any function. This numerical scheme implies that the condensation adjustment step is part of the iterative solution of the resulting implicit equation. The iteration stops whenever the new estimate of the temperature is closer than 0.001 K to the last estimate. The integration from 1000 to 100 mb takes 600–900 steps with a mean pressure increment $\Delta P \approx 0,5 \text{ mb}$. The total simulated duration of the parcel ascent (or descent) is about 25 min with the vertical velocity specified by (23).

For each parcel predictive quantity (potential temperatures or enthalpy), the same semi-implicit integration scheme of its rate of change equation [(16) and (22)] is set up in order to predict its new value at the level $P + \Delta P$. The value of the ice-liquid potential temperature changes only under the influence of liquid water and ice unloading due to its extensive property (Tripoli and Cotton, 1981). In each case, the values of the rain, ice, graupel and total mixing ratios are assumed to be given by the referenced values obtained during the integration process of the basic equation. The values of the temperature, the cloud water and water vapor mixing ratios, the air density and the altitude are obtained each time as results of the inversion of each predictive quantity. Educated guess values of the above parameters are assumed, except the temperature, which is deduced from the value of the predictive quantity. A new estimate of the other parameters is deduced from the temperature, the saturated vapor mixing ratio and all the "referenced" values.

Three cases have been considered in the numerical simulations:

CASE I. The terminal velocity of rain and graupel particles is set equal to zero and the total mixing ratio is constant. In this case, all the predictive quantities (potential temperatures or enthalpy) happen to stay constant. This case will tend to overestimate the errors since the condensate mixing ratio can reach a value of 0.02 which is seldom reached inside real clouds.

CASE II. The terminal velocities are functions of the mixing ratios but the total mixing ratio remains constant. Here terms like $V_h \cdot \nabla T$ are taken to be identical in all four integrations. The comparison of this case to case I will give an indication of the order of magnitude of the last two terms of (1) which have usually been neglected previously (except for Das, 1969). These terms describe the cooling of the air due to the effect of the downward flux of cooler precipitating particles. Since the precipitation mixing ratios are too high due to the absence of fallout mechanisms, the consequences of these terms will be slightly overestimated.

CASE III. The total mixing ratio decreases due to the precipitation of rain and graupel particles, which is modeled by the arbitrary equations

$$\left. \begin{aligned} \frac{dr_r}{dt} &= -r_r/\tau \\ \frac{dr_h}{dt} &= -r_h/\tau \end{aligned} \right\} \quad (26)$$

where $\tau = 2000$ s is a relaxation time chosen to be larger than the total time for the parcel rise or descent. In this case, the error should be underestimated since no processes of rain accumulation have been considered and the rain and graupel mixing ratios can be very small.

4. Results of the simulations

a. Case I

The potential temperature errors are defined as the difference between the potential temperatures which are obtained from the use of the three predictive quantities (θ_{il} , θ_q , H_l) and the potential temperature of the parcel obtained as the result of the integration of the basic equation (1). These errors are shown, for case I, in Fig. 1a by the curves labeled 1-3 as functions of the parcel pressure during the rise of the parcel. The value of each mixing ratio is shown in Fig. 1b, as a function of the pressure, by the vertical distance between the two curves enclosing each domain during the rise of the parcel. Figs. 2a and 2b show similar results for a descending parcel. The lowest curves in Figs. 1b and 2b correspond to the water vapor mixing ratio and the dotted curve corresponds to their saturated values. During the rise of the parcel, these two curves are identical (Fig. 1b) while, during the descent (Fig. 2b), the relative humidity is indicated by the ratio of the distances between each curve and the axis, and can be as low as 15% for any pressure greater than 800 mb in case I. The total mixing ratio, which is indicated by the vertical distance between the highest curve in Figs. 1b and 2b and the axis, can be seen to stay constant in case I.

As shown in Fig. 1b during the parcel rise, the small droplets appear as soon as the parcel becomes saturated at about 850 mb, are changed by autoconversion into precipitating drops for pressures below 650 mb, and are completely frozen into small crystals for pressures below 180 mb. Precipitating drops grow by accretion of small droplets and by self-coalescence and start to freeze for pressures below 300 mb. Ice crystals, which originate from the freezing of small droplets, are accreted by raindrops and by precipitating graupel.

As shown in Fig. 2b, during the parcel descent, the

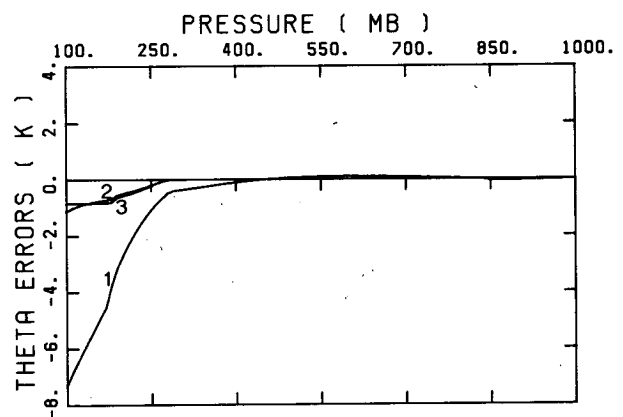


FIG. 1a. Potential temperature errors (K) for 1, the ice-liquid potential temperature, 2, the wet equivalent potential temperature, 3, the wet equivalent enthalpy, during parcel rise (from right to left) in case I as functions of the total pressure.

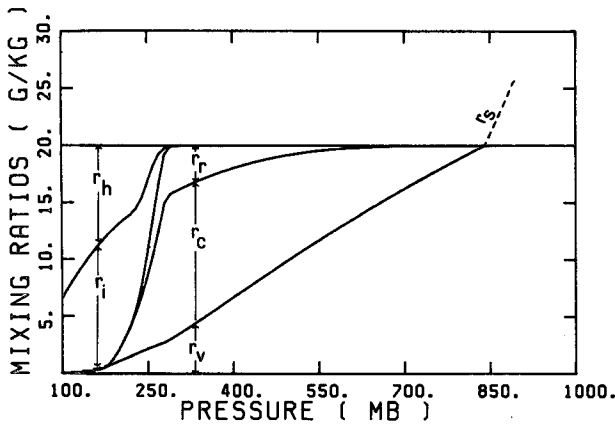


FIG. 1b. Mixing ratios versus pressure during parcel rise (from right to left) in case I.

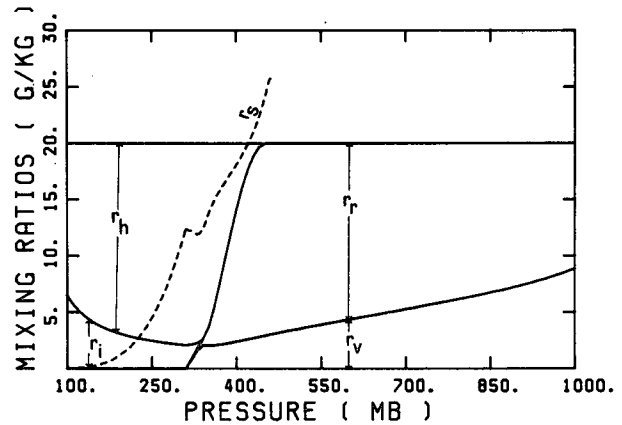


FIG. 2b. As in Fig. 1b except during parcel descent (from left to right) in case I.

precipitating graupel continue to accrete the small ice crystals and both species start to sublime in the unsaturated air. For pressure higher than 320 mb, ice crystals followed by precipitating graupel start melting into small droplets which evaporate instantaneously and into precipitating drops which evaporate slowly in the unsaturated air. The water vapor mixing ratio increases up to 0.0085 at 1000 mb and precipitating drops reach the ground.

During the first part of the parcel rise shown in Figs. 1a and b, the parcel temperature deduced from each conserved quantity is remarkably close to the "reference value" until the parcel reaches 300 mb (Fig. 1a) when ice particles appear (Fig. 1b). The potential temperature error levels off at a value of about 1 K for the temperature deduced from the wet equivalent potential temperature or the wet equivalent enthalpy, but reaches -7 K for the ice-liquid potential temperature.

During the parcel descent (Figs. 2a and b), the temperature errors for two predictive quantities increase below 300 mb due to the evaporation of raindrops in

the subsaturated air. However, the potential temperature deduced from the wet equivalent enthalpy becomes closer to the reference potential temperature and the errors become as low as 0.12 K, showing that this quantity can take into account the thermodynamic effects due to all the nonreversible phase changes. The wet equivalent and the ice-liquid potential temperatures can lead to errors of several degrees in the determination of the parcel potential temperature.

The numerical errors created by the integration of (1), (16) and (22) accumulate during the ascent and the descent. However, these numerical errors can be estimated by the wet equivalent potential errors and the wet equivalent enthalpy errors below 300 mb during the parcel rise since, in this case, the approximations are exact. Fig. 1a shows that these numerical errors are below 0.05 K between 1000 and 300 mb.

b. Case II

The curves corresponding to the parcel rise (not shown) are almost identical to those of Figs. 1a and 1b, since precipitating particles appear only above 600 mb. Figure 3a concerns the parcel descent and shows that, beside the curve relative to the ice-liquid potential temperature (curve 1) which rises up to 5 K, the potential temperature errors are almost identical to those of case I. Indeed, the rate of change equations for the wet equivalent potential temperature and for the wet equivalent enthalpy includes the cooling effect due to precipitation while, in this case, the ice-liquid potential temperature does not change since the total mixing ratio is kept constant. The mixing ratios are shown in Fig. 3b for the parcel descent. These curves indicate that the humidity is larger in case II than in case I for any pressure larger than 300 mb. This fact is due to the cooling of the air induced by the downward flux of precipitating particles (cooler particles) through the parcel.

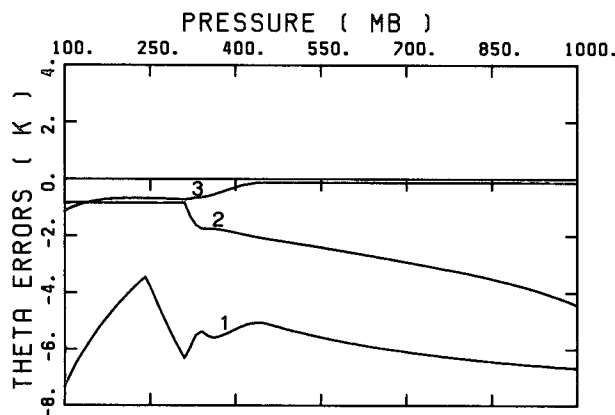


FIG. 2a. As in Fig. 1a except during parcel descent (from left to right) in case I.

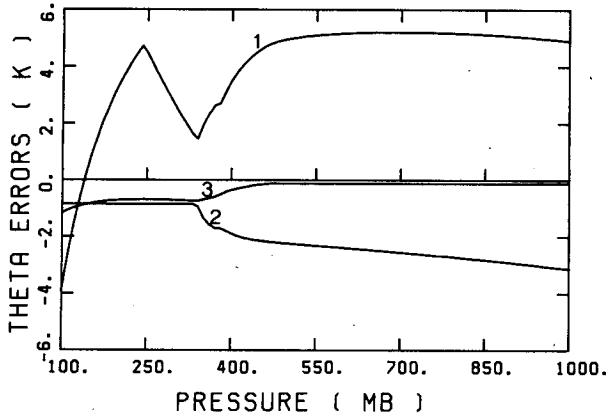


FIG. 3a. As in Fig. 1a except during parcel descent (from left to right) in case II.

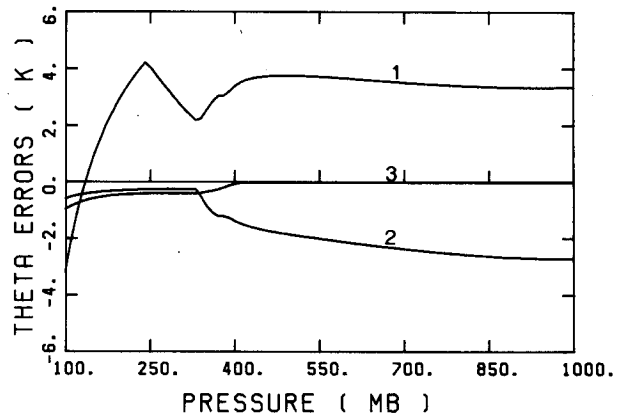


FIG. 4a. As in Fig. 1a except during parcel descent (from left to right) in case III.

c. Case III

The curves of the potential temperature errors as functions of pressure (not shown for the parcel rise and shown in Fig. 4a for the parcel descent) are almost identical to the corresponding curves for case I, even if the magnitude of the errors is slightly less in this case. The total mixing ratio decreases from 20 g kg^{-1} to 16.8 g kg^{-1} during the parcel rise and, as shown in Fig. 4b, decreases further to 11.4 g kg^{-1} during the parcel descent. Due to the inclusion of a precipitation process, the mixing ratio for precipitating drops and ice particles are smaller in this case than in case I or II. This implies that the potential temperature errors which are mainly caused by the nonreversible evaporation process of ice and rain particles and by the precipitation process are less important than in case I or II.

For the choice of a predictive quantity to be used in the simulation of atmospheric flows, two aspects

must be considered. The first is the errors of the simulation and has been treated above. The second aspect is concerned with the coupling between the thermodynamical, microphysical and kinematical (continuity) equations. This coupling is the weakest when the change in the predictive quantity is small; that is, when its new value is close to its old value during the integration.

The changes in the predictive quantities during the parcel descent are shown in Fig. 5 as functions of the pressure. The change in the wet equivalent enthalpy is expressed in kelvins obtained by dividing it by the specific heat C_{pd} of dry air at constant pressure. The largest values of the change in the predictive quantities are approximately 25.4 K, -0.7 K and 16 K for the ice-liquid potential temperature, for the wet equivalent potential temperature and for the wet equivalent enthalpy, respectively. Curve 2 in Fig. 5 suggests that, in this case, with very small errors, the wet equivalent potential temperature can be assumed to be constant

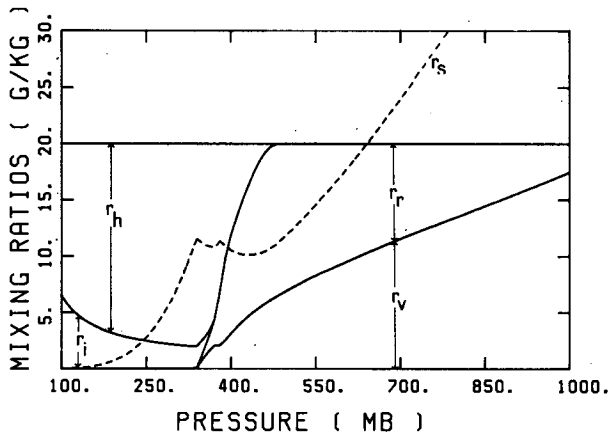


FIG. 3b. As in Fig. 1b except during parcel descent (from left to right) in case II.

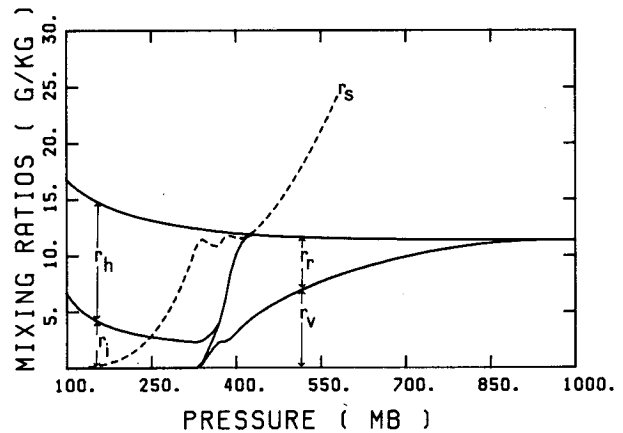


FIG. 4b. As in Fig. 1b except during parcel descent (from left to right) in case III.

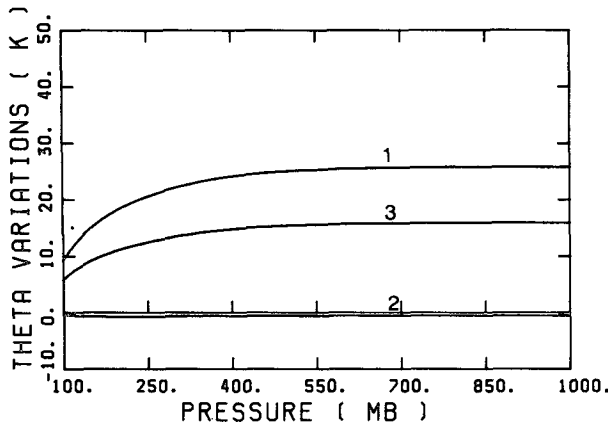


FIG. 5. Variation of 1, ice-liquid potential temperature (K), 2, wet equivalent potential temperature (K), 3, wet equivalent enthalpy (K) (divided by C_{pd}), as functions of parcel pressure (mb) during parcel descent in case III (from left to right).

following the parcel path. In all circumstances, the variations of WEPT are small and are due only to precipitating particles.

5. Discussion and conclusions

This work emphasizes the thermodynamical consequences of such nonreversible phenomena as freezing of supercooled water, evaporation in undersaturated air and precipitation processes. A basic thermodynamical equation is given which involves all the terms considered both by Das (1969) and Tripoli and Cotton (1981). This equation relates the rates of change of temperature, pressure and mixing ratios under all circumstances, even when nonreversible phase changes are involved and equilibrium is not assumed.

Two predictive quantities (WEPT, WEE) are proposed which are analogous to the ice-liquid potential temperature proposed by Tripoli and Cotton for use in numerical models. Any of these quantities, together with the total mixing ratio, can serve as prognostic variables in numerical models instead of the temperature, the total mixing ratio and the water vapor (or droplet) mixing ratio. The use of these predictive quantities avoids the need of a saturation adjustment step and can decrease by one the number of prognostic variables. The actual water vapor or the droplet mixing ratio are simply diagnosed from the new values of the predictive quantity and of the total mixing ratio. All the predictive quantities considered in this work are constant when precipitating particles are absent and their rate of change equations are given whenever precipitating particles appear.

Simple computation with Lagrangian parcel models suggests that the errors are larger when the ice-liquid potential temperature is used than when the wet equivalent potential temperature is used. For both potential

temperatures, the errors are larger (up to 5 K) when supercooled particles freeze and when precipitating drops or precipitating ice particles evaporate in non-saturated air. The important advantages of the wet equivalent potential temperature lie in the fact that it can be used in nonhydrostatic flows and its value changes only in the presence of precipitating particles. The largest errors arise when evaporation of particles occurs in nonsaturated air. However, the errors are smaller than when the ice-liquid potential temperature is used. The main drawback of this potential temperature comes from the rather lengthy computational scheme associated with the inversion of its value.

The use of the wet equivalent enthalpy also leads to very small errors, less than 1 K, and occurs when supercooled particles freeze. The fact that the rate of change of the pressure appears in the equation for the rate of change of the wet equivalent enthalpy is not a serious drawback for using this predictive variable since, as discussed by Tripoli and Cotton (1981), the coupling between the thermodynamical equation and the continuity equation or the pressure tendency equation exists for any predictive quantity. Furthermore, a nonhydrostatic pressure perturbation at the ground of as much as 10 mb leads to a change in the wet equivalent enthalpy of less than 1 K which is small compared to the change induced by the precipitation process as shown in Fig. 5. The prediction of temperature, therefore, is not very sensitive to the nonhydrostatic pressure term. It should be accurate enough to estimate the pressure to be used in (22) without taking into account the influence of the unknown change in temperature. The new pressure can then be calculated by using this predicted value of the temperature. Since the wet equivalent enthalpy is mostly quadratic in the independent variables, its inversion can be done on a digital computer with competitive speed. Therefore, the wet equivalent enthalpy should be very useful in the numerical simulation of atmospheric flows by allowing the modeler to take a more complete account of the thermodynamical and dynamical effects of the water species.

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APPENDIX

List of Symbols

A_{lv}, A_{il} affinity of vaporization and of melting ($J\ kg^{-1}$)

$C_i, C_l,$ C_{pd}, C_{pv}	specific heats at constant pressure of ice, liquid water, dry air and water vapor ($J K^{-1} kg^{-1}$)	w	vertical component of the velocity vector ($m s^{-1}$)
C_{pt}	mean specific heat at constant pressure of cloudy air ($J K^{-1} kg^{-1}$)	z	vertical coordinate (m)
d	suffix for dry air	γ	ratio of the specific heats of dry air
e_i	saturated partial pressure of water vapor over a plane ice surface (mb)	ϵ, ϵ'	ratios of the molecular weight and of the specific heat of water vapor to those of dry air
e_v, e_s	partial pressure of water vapor and its sat- urated value (mb)	$\rho_d, \rho_i, \rho_l,$ ρ_v, ρ_T	density of dry air, ice particles, liquid water, water vapor and total density ($kg m^{-3}$)
g	acceleration due to gravity ($m s^{-2}$)	$\theta, \theta_{il}, \theta_q$	dry air, ice liquid and wet equivalent potential temperature (K)
h_i, h_v, h_l	enthalpy of ice, of water vapor and of liquid water ($J kg^{-1}$)	χ	any variable
Hl	wet equivalent enthalpy ($J kg^{-1}$)	τ	relaxation time (s).
i	suffix for ice particles		
l	suffix for liquid water		
L_{il}	latent heat of melting ($J kg^{-1}$)		
L_{lv}	latent heat of vaporization ($J kg^{-1}$)		
L_1, L'	equivalent latent heat due to the vaporiza- tion in undersaturated air and to the freezing of supercooled drops ($J kg^{-1}$)		
M_d, M_v	molecular weight of dry air and water vapor (kg)		
P, P_d	total pressure and partial pressure of dry air (mb)		
q_c	specific condensate content [$=(\rho_l + \rho_i)/\rho_T$]		
$r_T, r_c, r_l,$ $r_r, r_i,$ r_h, r_v	total water mixing ratio, condensed wa- ter mixing ratio, liquid water mixing ratio, raindrop mixing ratio, ice mix- ing ratio, hail mixing ratio and water vapor mixing ratio		
R_d, R_v	gas constants for dry air and water vapor ($J K^{-1} kg^{-1}$)		
$s_d, s_i, s_l,$ s_v	specific entropy of dry air, ice particles, liquid water and water vapor ($J K^{-1}$ kg^{-1})		
T, T_l, T_i	air temperature, drops temperature and ice particles temperature (K)		
u	velocity vector ($m s^{-1}$)		
v	suffix for water vapor		
V_i, V_h, V_l	terminal velocity of ice particles, of hail and of water drops ($m s^{-1}$)		

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