

Continuity equations as expressions for local balances of masses in cloudy air

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ABSTRACT

The mathematical representation of the mass continuity equation and a boundary condition for the vertical velocity at the earth's surface is re-examined in terms of its dependence on the frame of reference velocity. Three of the most prominent meteorological examples are treated here: (a) the barycentric velocity of a full cloudy air system, (b) the barycentric velocity of a mixture consisting of dry air and water vapour and (c) the velocity of dry air. Although evidently the physical foundation holds independently of the choice of a particular frame, the resulting equations differ in their mathematical structure: In examples (b) and (c) the diffusion flux divergence that appears in the corresponding mass equation of continuity should not be omitted a priori. As to the lower boundary condition for the normal component of velocity, special emphasis is placed on the net mass transfer across the earth's surface resulting from precipitation and evaporation. It is shown that for a flat surface, the reference vertical velocity vanishes only in case (c). Regarding cases (a) and (b), the vertical reference velocities are determined as functions of the precipitation and evaporation rates. They are nonzero, and it is shown that they cannot generally be neglected.

1. Introduction

Mathematical models with which the spatial-temporal behaviour of the atmosphere can be analyzed and predicted are commonly established using the fundamental physical budget criteria for matter (related to both the total mass of cloudy air and its partial component masses) as well as momentum and internal energy coupled with the thermodynamic equation of state. The formulation of local differential equations from global (integral) balance criteria makes it necessary to fix a reference velocity to which the diffusion or relative transport velocities of the system's constituents are referred (e.g. Haase, 1990, or Gyarmati, 1970 explore this matter instructively). The formulation of the general set of thermo-hydrodynamic equations for the

modelling of cloudy air convection has recently been reinspected by Bannon (2002).

In the case of a multiphase and -component system such as cloudy air, the appropriate reference velocity is frequently assumed to be the barycentric velocity of all contributing substances (dry air + water vapour + water condensate), termed the total system, or merely the barycentric velocity of the gas mixture consisting of dry air + water vapour, or even the dry air component velocity.

It is to be expected that the formal representation of the resulting basic differential equations is not independent of the chosen reference velocity, although the physical background may evidently not be effected by that. So for instance, divergence terms of diffusion fluxes would, in contrast to its familiar formulation, immediately show up in the mass equation of continuity, if the component velocity of dry air is introduced as reference velocity; this aspect is discussed in Section 3.

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The use of hydro-thermodynamic differential equations for model simulations of the atmosphere requires definition of relevant boundary conditions. In the case of mass fluxes, it is suitable to assume that no mass leaves the atmosphere at its upper boundary surface. On the other hand, to model a physically reasonable lower boundary for the earth's surface, one assumes that a relevant velocity component, directed normally to the boundary, has to vanish,

$$\mathbf{v}_s \cdot \mathbf{n} = 0. \quad (1)$$

Here \mathbf{v}_s denotes the surface velocity vector and \mathbf{n} the surface-normal unit vector. A similar boundary concept is employed e.g. by Doms and Schättler (1999) in their analysis of the framework equations of the high resolution weather prediction model of the DWD (German Weather Service).

Note that if the velocity vector \mathbf{v} in eq. (1) is defined as the barycentric velocity of the dry air + water vapour + water condensate mixture, the boundary condition means that the net mass flux across the ground surface has to go to zero. This postulate does not imply that the atmosphere is a (materially) closed system, but should be interpreted as a side condition for the sum of mass fluxes across the surface boundary. Actually, the real physical situation is that mass transports of water vapour and of water condensate across the surface by evaporation and precipitation are ubiquitous, while mass transports of dry air may result from emissions of CO_2 or exhalations of other trace gases as well as wash-out of (dry) aerosol particles; however, these contributions from external sources of dry air are so small that they can be disregarded. Therefore, as a more appropriate quantity, the dry air velocity \mathbf{v}_0 should rather be associated with the ground surface condition, i.e.

$$\mathbf{v}_{0s} \cdot \mathbf{n} = 0 \quad (2)$$

which, from a meteorological point of view, characterizes the model's lower boundary better than eq. (1).

Non-negligible contributions to the mass flux across the ground surface are provided by transports of H_2O as a result of precipitation and evaporation or dew formation. As a consequence, the boundary condition (1) is only satisfied if the rates of evaporation/dew formation and of precipitation compensate at each location for all times, which does not, however, hold true in the atmosphere. Indeed, not even in a climatological mean do the rates of evaporation and precipitation coincide for most areas. This fact is then disregarded if it

is assumed that the total barycentric velocity vanishes with eq. (1) at the lower boundary.

There are only sporadic hints at inconsistencies in common formulations of the mass balance in the literature: Saito (1998), for instance, addresses the sensitivity of model results on the formulation of the continuity equation. Trenberth (1991) and Trenberth et al. (1995) hint at some inconsistencies in the formulation of the mass balance, but unfortunately do not distinguish strictly between total air mixture and the gas mixture, so that not all inconsistencies are removed in their studies of imbalances in the mass field for climatological purposes, arising from numerical effects in analyzed global data. Moreover, in a study on vertical fluxes in the surface layer, Bernhardt (1989) considers a non-zero advective mass flux caused by evaporation at the surface. A systematic investigation of the effect of the approximative boundary conditions (1) on the mass balance is, to the authors' knowledge, presently not available.

To clarify the origin of different formulations of the mass balance in the literature [see e.g. Bannon (2002), Doms and Schättler (1999) and Saito et al. (2001)], the continuity equation of mass and the appropriate lower boundary condition for the vertical velocity are formulated and discussed in this paper for three cases of the reference velocity, and the matching boundary condition for the mass transfer.

This compilation also contributes to the derivation of a correct description (within the frame of the above assumptions) of the mass balance in model equations, as is necessary for all numerical simulations ranging from models for mesoscale processes with high local precipitation and evaporation to models for global climate simulations.

2. Model assumptions and related basic laws

As a model for the atmosphere which is sufficiently simple to be taken as a basis for setting up practical local mass balance equations in Section 3, we consider a mixture of gaseous constituents, that are dry air (index 0) and water vapour (index 1), as well as water condensate particles (index 2). Henceforth, these three constituents will be loosely referred to as mass components; here this is a practical definition, since we need an abstract simplification of the physico-chemical composition. In this way, we avoid investigation of a system consisting of a gaseous molecular component in which liquid and solid phase

hydrometeors are distributed similar to a suspension. Dry air is treated as chemically inert and as a homogeneous component, and any transfer of dry air across the earth's surface is disregarded; hence, total mass of dry air in the atmosphere is taken to be constant. Take a component k with mass M_k in a volume V and partial density ρ_k ; then the relation

$$M_k = \int_V \rho_k dV \quad (3)$$

is true for $k = 0, 1, 2$. Based on physical evidence, it follows that for the mixture of components the total mass M and density ρ are obtained by summing the corresponding partial quantities of all components:

$$\rho = \sum_k \rho_k, \quad M = \sum_k M_k = \int_V \rho dV. \quad (4)$$

The partial mass M_k of a continuous system with fixed volume V is changed by mass fluxes across the boundary area of V as well as by internal local sources, as e.g. provided by H_2O transformations in form of growth or decay of drops by condensation or evaporation, respectively. In order to be able to capture such effects explicitly, one needs a locally valid mathematical framework. This is obtained by a differential transformation of the global balance criterion for an M_k -mass to an equivalent local balance equation for M_k 's partial density function ρ_k . We then arrive at the equation of continuity for a partial mass component (see the note at the end of this section):

$$\frac{\partial \rho_k}{\partial t} = -\nabla \cdot \mathbf{F}_k + \sigma_k \quad (\forall k). \quad (5)$$

In eq. (5) the vector of the divergence term is the expression

$$\mathbf{F}_k = \rho_k \mathbf{v}_k \quad (6)$$

which denotes the individual mass flux density of a component k , wherein the transport speed vector \mathbf{v}_k is the mean component velocity. In eq. (5) the companion term σ_k denotes the conjugated internal production rate; the sum of all σ_k -sources vanishes,

$$\sum_k \sigma_k = 0, \quad (7)$$

which reflects the fact that chemical reactions and transitions among the mass components do not affect changes of the total mass.

Some special physico-chemical conditions of our model atmosphere are to be examined. For a non-reactive substance like dry air, the source strength rate

identically vanishes, $\sigma_0 = 0$. The water vapour and condensate source rates σ_1 and σ_2 , respectively, account for phase changes by condensation/evaporation and deposition/sublimation, and are therefore non-vanishing terms; they sum up to zero ($\sigma_1 + \sigma_2 = 0$) in agreement with the conservation of total H_2O mass.

In general, the component velocities \mathbf{v}_k are all different. Hence we observe not only a macroscopic motion of all mass components with a reference velocity \mathbf{v}_r , which is specified later, but also a motion of each component relative to \mathbf{v}_r , i.e. $\mathbf{v}'_k := \mathbf{v}_k - \mathbf{v}_r$. The reference velocity \mathbf{v}_r should be defined as some mean value of the component velocities. In geophysical fluid systems, this reference velocity is frequently chosen as the barycentric, i.e. mean mass weighted velocity of the system,

$$\mathbf{v} := \sum_{k=0}^2 m_k \mathbf{v}_k. \quad (8)$$

Formula (8) has the mass fractions $m_k := \rho_k / \rho$ as weighting factors for the partial velocity vectors. It holds the ultimate m_k -condition $\sum_k m_k = 1$, in full equivalence with eq. (4). In reference to barycentric motion, we can then define the corresponding mass diffusion flux vectors

$$\mathbf{J}_k = \mathbf{F}_k - \rho_k \mathbf{v} = \rho_k (\mathbf{v}_k - \mathbf{v}). \quad (9)$$

From eq. (9) together with eq. (8) one easily verifies the validity of the sum condition

$$\sum_{k=0}^2 \mathbf{J}_k = 0, \quad (10)$$

which must necessarily be satisfied by the \mathbf{J}_k -vectors independent of the dynamic situation of the fluid.

For special conditions of the system under consideration, concentrations such as mole fractions or volume fractions [see Haase (1990) and Herbert (1980)] can be more appropriate than the mass fractions m_k for utilization in eq. (8), and they result in a reference velocity which is different from the barycentric one.

For particular purposes, however, it may be appropriate to employ, as a modification to eq. (8), a reference velocity which does not account for all mass flux contributions. Sometimes, for instance, it is sufficient to adopt as reference velocity either the component velocity of dry air

$$\mathbf{v}_r = \mathbf{v}_0 \quad (11)$$

or, if a mixture of dry air and water vapour has been chosen as reference frame, the barycentric gas mixture

velocity, i.e.

$$\mathbf{v}_r = \mathbf{v}_g := q_0 \mathbf{v}_0 + q_1 \mathbf{v}_1; \quad (12)$$

note that this concept involves weighting factors in form of the concentrations $q_k := \rho_k / \rho_g$, with $\rho_g := \rho_0 + \rho_1$ denoting the density of the gas mixture.

To complete this section a description of the component velocity of the condensate, which is composed of an ensemble of condensate particles, is given. We will interpret the barycentric average velocity of the particle population as component velocity \mathbf{v}_2 . Insofar as the condensate mainly consists of large precipitating particles as in case of rain below a cloud, then the difference of the vertical motion of precipitating particles from the barycentric velocity of air can be approximated with high accuracy by the so-called sedimentation or terminal fall velocity according e.g. to the treatise of Rogers and Yau (1989). Since sedimentation of large particles is the most important contribution to the vertical component of the condensate diffusion flux J_2^z , we can approximate J_2^z by the downward directed mass flux P as a result of precipitation (or sedimentation), that is $J_2^z \approx -P$.

To simplify matters, in the following we also assume a flat surface. The results, however, can be easily transferred to more general surface conditions. The vertical component of a vector will be henceforth denoted by an upper index z .

Note to the text: A main objective of the thermodynamic theory of continuous systems is to develop field differential equations, the so-called equations of continuity, with concern to extensive variables of state such as mass, momentum, energy, entropy, etc. Let A denote an arbitrary extensive variable of state belonging to a volume V , and α the density function as well as a the specific function of A , which are both specified at each point in V and on its surface area. Then from global criteria connected with A , one derives the general equation of continuity,

$$\frac{\partial \alpha}{\partial t} = -\nabla \cdot \mathbf{F}_A + \sigma_A \quad (13)$$

or alternatively

$$\frac{\partial \rho a}{\partial t} = -\nabla \cdot \mathbf{F}_A + \sigma_A, \quad (14)$$

where α , a , ρ , as well as \mathbf{F}_A and σ_A depend on time and position. The differential operator $\partial/\partial t$ denotes the derivative with respect to time at fixed position and $\nabla \cdot$ the divergence derivative with respect to the position coordinates. It is physically justified to consider

the field equation (13), and also the equivalent (14), as a local balance of the state function A . This interpretation is based on the relationship that, in agreement with the integral definition $A = \int_V \alpha \, dV = \int_V a \rho \, dV$, each differential volume provides a contribution to the local rate of change of A as a result of the behaviour of its local density or specific function, respectively.

In the above theorem of continuity, the divergence term $\nabla \cdot \mathbf{F}_A$ (with its dependence on the efficiency and direction of the current density \mathbf{F}_A) represents the external 'source' strength density of A , flowing out of a differential volume through its bounding surface. The term σ_A , called the local production of A , expresses the interior differential contribution of a unit volume element to the total production of A inside the whole volume V .

Here the case we consider with $\alpha \equiv \rho_k = m_k \rho$, i.e. $a = m_k$, is the class of mass equations of continuity as expressions of local mass balances in a multi-component continuous system.

3. Continuity equation of mass and lower boundary condition

In this section, mass balances and lower boundary conditions for the vertical reference velocity w_r are formulated for three reference systems which are common in meteorology; they have already been addressed in the previous section.

3.1. Barycentric velocity of the total air mixture

To begin with, the full barycentric velocity (8) is utilized as reference velocity. By use of eq. (9), the local balance equation (5) of a mass component k then transforms to

$$\frac{\partial \rho_k}{\partial t} = -\nabla \cdot (\rho_k \mathbf{v} + \mathbf{J}_k) + \sigma_k, \quad (15)$$

wherein \mathbf{J}_k is the diffusion flux, and $\rho_k \mathbf{v}$ is the advective mass flux in the barycentric reference frame.

Summing up in eq. (15) over all components $k = 0, 1, 2$ with regard to the mass control conditions (4), (7) and (10) the result is the total mass equation of continuity,

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}). \quad (16)$$

For the sake of simplicity, we assume in this paper a flat surface. The lower boundary condition used in

atmospheric models is often a representation of an impermeable ground surface with respect to dry air mass. That is, we may postulate that the vertical dry air density flux component, normal to the earth's surface, becomes zero at the boundary,

$$(\rho_0 w_0)_s = 0. \quad (17)$$

In contrast, the mass density fluxes of water vapour and water condensate across the boundary surface do not vanish, since evaporation of liquid water and sublimation of ice from the soil or ocean take place, as does precipitation from clouds:

$$(\rho_1 w_1)_s \neq 0, \quad (\rho_2 w_2)_s \neq 0. \quad (18)$$

Hence, from eq. (8) in agreement with the three criteria in eqs. (17) and (18), then immediately follows the formula

$$w_s = (m_1 w_1)_s + (m_2 w_2)_s \quad (19)$$

for the vertical boundary barycentric velocity normal to the surface. In order to make the natural relevance of the w_s -relation in its physical sense more transparent, recall that the right-hand side sum in eq. (19) can be substituted by the corresponding vertical components of the diffusion flux densities which are associated with eq. (9). Doing that, and also introducing the vertical vapour diffusion density flux (E) as well as the precipitation density flux (P) via the notation $J_1^z = E$ and $-J_2^z = P$, respectively, eq. (19) then transforms to the w_s -expression

$$w_s = \left(\frac{E - P}{\rho m_0} \right)_s. \quad (20)$$

From eq. (20) it follows that only if the fluxes of precipitation and evaporation at the ground surface can be assumed to be nearly in balance, can one speak of a boundary condition $w_s = 0$. Such a situation at the atmosphere–earth boundary requires, of course, very special physical circumstances, and thus generally can not hold. Also in a climatological mean for a certain region, one will rather observe a net mass transport across the lower boundary associated with a normal barycentric velocity component. As a consequence of that, a relevant dynamical contribution to the surface pressure tendency $\partial p_s / \partial t$ will arise. Here we consider the corresponding $\partial p_s / \partial t$ -equation in relation to flat bounding terrain as well as hydrostatic conditions via

$\partial p / \partial z = -g\rho$; it then takes the form

$$\begin{aligned} \frac{\partial p_s}{\partial t} &= -g \int_{z_s}^{\infty} \nabla \cdot (\rho \mathbf{v}_h) dz + g[\rho w]_s \\ &= -g \int_{z_s}^{\infty} \nabla \cdot (\rho \mathbf{v}_h) dz + g \left(\frac{\rho}{\rho_0} (E - P) \right)_s, \end{aligned} \quad (21)$$

in which \mathbf{v}_h denotes the barycentric velocity vector with respect to horizontal directions. Imbalances of the diffusion fluxes of water vapour and precipitation in eq. (21) are simply involved via the second term of the sum on its right-hand side. As result of their formulation, they describe direct boundary surface effects, i.e. they are independent of (integral) contributions of the air column above it, and they vanish immediately in the case of a materially closed surface.

Note clearly in that context the formal dependence on the physical relevance of the E - and P -terms which, in the above representation, have been postulated as pure diffusion effects [associated with eq. (20)]. If in another sense E - and P -expressions had been introduced, for instance, as total mass fluxes, i.e. including advective and diffusive parts, as it is frequently found in the literature, then it can be shown that the factors ρm_0 in eq. (20) and ρ / ρ_0 in eq. (21) have to be replaced by ρ and 1, respectively.

It should be also noticed, that if in the differential relation of hydrostatic equilibrium the density ρ is substituted by the gas mixture density ρ_g alone, one obtains, in modification of eq. (21), the following p_s -integro-differential equation:

$$\begin{aligned} \frac{\partial p_s}{\partial t} &= -g \int_{z_s}^{\infty} \nabla \cdot (\rho_g \mathbf{v}_h) dz + g[\rho_g w]_s + g P_s \\ &\quad - g \int_{z_s}^{\infty} \sigma_2 dz \\ &= -g \int_{z_s}^{\infty} \nabla \cdot (\rho_g \mathbf{v}_h) dz + g \left(\frac{\rho_g}{\rho_0} (E - P) \right)_s \\ &\quad + g P_s - g \int_{z_s}^{\infty} \sigma_2 dz. \end{aligned} \quad (22)$$

Hence additional terms related to the condensate mass turn up. Let us assume that as soon as condensate is formed in a column of air, it instantaneously falls out to yield the surface precipitation rate P_s , we have $\int_{z_s}^{\infty} \sigma_2 dz = P_s$, and therefore the last two terms in the tendency equation (22) drop out. Because a model state like that disregards the explicit existence of condensate water mass as part of the atmosphere, it is

consequent to apply the density approximations $\rho_2 = 0$ and $\rho = \rho_g$ in eq. (21), which then agrees with eq. (22).

As to the diffusion flux J_0^z of dry air at the surface, it does not vanish; its occurrence is necessary to compensate for the transport of dry air brought about by the barycentric velocity w_s as to fulfil the natural condition $(F_0^z)_s = 0$.

3.2. Barycentric velocity related to the gas mixture

In the second case, the barycentric velocity \mathbf{v}_g related to the gaseous dry air + water vapour mixture will be employed as reference velocity; see eq. (12). The total mass flux of component k , see eq. (6), can then be written as

$$\mathbf{F}_k = \rho_k \mathbf{v}_g + \mathbf{J}_{k,g}. \quad (23)$$

Equation (23) accords with the diffusion flux representation

$$\mathbf{J}_{k,g} := \rho_k (\mathbf{v}_k - \mathbf{v}_g), \quad (24)$$

and thus, from eq. (23) as from eq. (24) one is led to the following relationship between the dry air and water vapour diffusion fluxes:

$$\mathbf{J}_{0,g} + \mathbf{J}_{1,g} = 0. \quad (25)$$

Hence, summing over $k = 0, 1$ in eq. (5) and accounting for eqs. (23) and (25) provides the following continuity equation for the mass of the two-component gaseous mixture:

$$\frac{\partial \rho_g}{\partial t} = -\nabla \cdot (\rho_g \mathbf{v}_g) + \sigma_1. \quad (26)$$

In contrast to the system's total mass equation of continuity (16), the continuity equation of the gas mass (26) depends on internal sources via σ_1 , i.e. the rate of phase change between water vapour and its condensate by condensation/evaporation or deposition/sublimation.

It evidently follows also that the \mathbf{v}_g -representation of the total mass equation of continuity remains free of σ -terms, i.e.

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}_g) - \nabla \cdot \mathbf{J}_{2,g}. \quad (27)$$

On the other hand, in contrast to the flux free barycentric representation (16), the continuity equation (27) separates the $\mathbf{J}_{2,g}$ -flux divergence. Assume that water vapour transport at the lower boundary yields the vertical velocity

$$w_{g,s} = (q_1 w_1)_s = \left(\frac{E_g}{\rho_0} \right)_s \quad (28)$$

with $E_g := J_{1,g}^z$. Then $w_{g,s} = 0$ holds only in the absence of evaporation and dew formation at the earth surface.

3.3. Velocity of dry air

Now the velocity of dry air \mathbf{v}_0 is taken as reference velocity. In that frame, the total mass flux \mathbf{F}_k of component k [see eq. (6)] is expressed as

$$\mathbf{F}_k = \rho_k \mathbf{v}_0 + \mathbf{J}_{k,0}, \quad (29)$$

wherein the relevant diffusion flux, now defined as $\mathbf{J}_{k,0} = \rho_k (\mathbf{v}_k - \mathbf{v}_0)$, vanishes for dry air. Therefore, the continuity equation of dry air mass is simply eq. (5) for $k = 0$ and $\sigma_0 = 0$:

$$\frac{\partial \rho_0}{\partial t} = -\nabla \cdot (\rho_0 \mathbf{v}_0). \quad (30)$$

One applies eqs. (4), (5) and (29) in a similar way to find the local balances of the other mass components; hence, these equations and eq. (30) can be summed up to give the following total mass equation of continuity

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}_0) - \nabla \cdot (\mathbf{J}_{1,0} + \mathbf{J}_{2,0}). \quad (31)$$

It is not surprising what eq. (31) shows as a result of the dry air reference frame: There are two diffusive flux divergences in the mass continuity equation, and this sum is generally different from zero. A real advantage of the choice of \mathbf{v}_0 as reference velocity is that the lower boundary condition for the reference velocity w_0 vanishes identically,

$$w_{0,s} = 0, \quad (32)$$

in agreement with the postulate that the lower boundary is impermeable to dry air. On the other hand, a severe disadvantage in the continuity equation (31) is the divergence contribution of diffusion fluxes in addition to the corresponding convective part coupled with the reference velocity \mathbf{v}_0 .

4. Discussion

In this study we have formulated local balance equations of air with respect to its total mass as well as partial mass components and considering three reference frames of velocity. Although the related continuity

equations (16), (27) and (31) express on the same physical basis the law of mass conservation, they differ in their structure. If the reference velocity is not chosen to be the barycentric velocity \mathbf{v} of the complete air mixture, but only parts of it, then a divergence of diffusion fluxes inevitably appears; moreover, it becomes obvious that the diffusion fluxes \mathbf{J}_k , $\mathbf{J}_{k,g}$ and $\mathbf{J}_{k,0}$ must differ. Corresponding additional divergence terms then do not occur, if the continuity equation is formulated in such a way that the relevant density is the particular density function, to which the reference velocity is related; i.e. ρ coupled with \mathbf{v} [see eq. (16)], ρ_g with \mathbf{v}_g [see eq. (26)] and ρ_0 with \mathbf{v}_0 [see eq. (30)]. Note that the continuity equation (26) in ρ_g -form contains a natural source rate, i.e. σ_1 for water vapour. A corresponding source rate σ_0 for dry air would likewise appear in eq. (26) and in the ρ_0 -form (30), if it were not set to be zero by definition.

Depending on the frame of reference, we found different lower boundary conditions for each of the relevant vertical velocities. The vertical reference velocity only vanishes correctly if it is chosen to be the velocity of dry air w_0 , see eq. (32), because the ground surface has been assumed to be a dry air - impermeable boundary. In the other frames of reference, the velocities w and w_g at the earth's surface are proportional to the difference between evaporation rate E and precipitation rate P , see eq. (20), and proportional to E_g , see eq. (28), respectively; hence they can only vanish in very special situations.

Apart from our special considerations, note that, like the total mass equations of continuity, all other thermohydrodynamic balance equations are formulated in dependence on a defined reference frame of velocity. For the differing diffusion fluxes \mathbf{J}_k , $\mathbf{J}_{g,k}$ and $\mathbf{J}_{0,k}$, correct parameterization equations are to be used, while the Fickian diffusion law, which is a good approximation for \mathbf{J}_k , cannot simply be adopted for $\mathbf{J}_{g,k}$ and $\mathbf{J}_{0,k}$.

For conditions as they are given in the natural atmosphere, H_2O contributions to the total air mass are small; $\rho_0 \gg \rho_1 \gg \rho_2$ even holds in many atmospheric situations. This relation justifies neglecting the numerical differences between ρ , ρ_g and ρ_0 and between \mathbf{v} , \mathbf{v}_g and \mathbf{v}_0 , only if the absolute values (and in case of the velocity also the direction) are of importance. Therefore one is frequently motivated to disregard any differences in those densities and velocities in the local mass balance equation and in the lower boundary condition for vertical velocity. The result of this is, however, violation of the exact balance of mass.

Two simple numerical examples will help to illustrate the order of magnitude of the vertical velocity at the surface:

(1) Suppose $m_0 \approx 1$ and $\rho \approx 1 \text{ kg m}^{-3}$, no evaporation, and a rain rate at the surface $P_s/\rho_w = 10 \text{ mm h}^{-1}$ (with ρ_w the bulk density of liquid water). This precipitation flux entails a net loss of mass in the atmosphere associated with a downward barycentric velocity of $w_s \approx -2.8 \text{ mm s}^{-1}$ [involving eq. (20)] as well as a reduction of the surface pressure of about 1 hPa within 1 h [involving eq. (21)]. That is, relative to the synoptic scale, vertical velocities and pressure tendencies of these orders are a priori not to be omitted.

(2) The Europa-Modell of the DWD simulated for the whole month July 1998 a mean rain rate of 1.4 mm d^{-1} and an evaporation rate of $2 \times 10^{-5} \text{ kg m}^{-2} \text{ s}^{-1}$ over the ocean-covered part of the model area (cf. DWD, 1998); here the evaporation rate is to be interpreted as the diffusive flux of water vapour E , and its amount would correspond to a mean rain rate of 1.7 mm d^{-1} . For these conditions we find an upward velocity of $w_s \approx 3.5 \times 10^{-3} \text{ mm s}^{-1}$. Hence, there is a net mass transport from the ocean to the atmosphere in that month. Due to such a boundary effect, on average the atmosphere gains mass over a large region and a whole month. The gain of mass in that example corresponds to an additional increase of mean surface pressure of 0.9 hPa within that month.

These crude estimations suggest that deviations from the exact formulation of the mass balance criteria in terms of continuity equations and the surface boundary condition may have an effect on the simulated evolution of the atmosphere. In a study related to this subject, Saito (1998) discussed a simulation performed with the nonhydrostatic weather prediction model of the Meteorological Research Institute of Japan. The equations to be integrated are based upon the assumption that dry air and water vapour move at the same speed, $\mathbf{v}_0 = \mathbf{v}_1$, and this velocity is also applied to set the reference frame. The continuity equation formulated for the total density ρ then contains additionally the divergence of the sedimentation flux, but no water vapour flux divergence (Saito et al. 2001, and Saito, personal communication). In a case study for a squall line (Saito, 1998) the impact of precipitation corresponds to a mean surface pressure change of 2 hPa within 7 h forecast time, and this is without doubt a considerable effect on the mass balance.

A paper which addresses explicitly the effect of mass transfer on the vertical velocity at the surface is that of Bernhardt (1989), who employs \mathbf{v}_0 as reference velocity. In order to compute w_s , however, he merely counts evaporation effects, so that the model atmosphere will always gain mass and the barycentric motion will be upward, $w_s \geq 0$. Bernhardt concludes from that study that the adjoint nonzero advective mass flux may contribute to the total vertical transport in the atmospheric surface layer to a non-negligible amount.

The use of a correct formulation of the mass continuity equation along with the matching surface boundary condition for the velocity has consequences for the formulation of the other prognostic equations, because these are likewise affected by the transport of the relevant quantities across the surface. However, only by expensive numerical model experiments is it possible to quantify to what extent the use of the corrected mass balance will influence the model simulations.

So far, the discussion has been conducted without consideration of basic theoretical questions encountered in reviewing the systematic applicability of alternative frames of velocity. Since this study focusses on theoretical fundamentals of local atmospheric mass balances, there is no contradiction involved in the use of one of the alternative set of equations. In a more de-

tailed framework, in which the field balance equations of momentum, angular momentum, energy and entropy of the system are also enclosed, a clear physical preference is seen to exist for the barycentric frame of reference. That frame also allows a particularly convenient and transparent formal representation of the field equations of continuity. A central term within, which most effectively profits from the use of the barycentric momentum as a measure of reference, is the contribution of diffusional processes in the balance of entropy that explicitly expresses the second principle law of thermodynamics. The expedience of a barycentric representation in the diffusion theory applies to general conditions just as to a Fourier–Fick-type fluid system existing in mechanical equilibrium (relative to mass and heat transport) without frictional forces. That subject, with its relevance to atmospheric diffusion conditions, has been examined by Herbert (1980; 1983).

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