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Flux-conservative thermodynamic equations in a mass-weighted framework

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ABSTRACT

A set of equations, ready for discretization, is presented for the purely thermodynamic part of atmospheric energetics along a vertical column. Considerations of kinetic energy budgets and detailed turbulence laws are left for further study. The equations are derived in a total mass-based framework, both for the vertical coordinate system and for the conservation laws. This results in the use of the full barycentric velocity as the vector of advection. Under these conditions, the equations are derived from first principles on the basis of an a priori defined set of simplifying hypotheses. The originality of the resulting set of equations is twofold. First, even in the presence of a full prognostic treatment of cloud and precipitation processes, there exists a flux-conservative form for all relevant budgets, including that of the thermodynamic equation. Secondly, the form of the state law that is obtained for the multiphase system allows the flux-conservative form to be kept when going from the hydrostatic primitive equations system to the fully compressible system and projecting then the heat source/sink on both temperature and pressure tendencies.

1. Introduction

The process leading to a set of equations for a physical phenomenon that one wishes to simulate is in general well codified. One starts from a well-agreed subensemble of the known laws of nature. One chooses a set of simplifying hypotheses. One sets a framework ensuring consistency of the mathematical derivation process (preservation of known invariants, use of conservation laws, etc.). One finally verifies that the result can lead to a 'model' of the phenomenon. Such is indeed the way in which the adiabatic part of most simulation models of the atmosphere is nowadays constructed. But, paradoxically, the diabatic part of the same models seldom has a set of governing equations built on the basis of similar sound scientific principles. In our opinion, this has happened because:

– 'plug-compatibility' was once an important goal, but it led to the belief that exchangeability was more important than consistency;

– some parametrization packages were developed under constraints only imposed by the dynamical core of their particular host model;

– the evolution of knowledge on which aspects of atmospheric behaviour can be meaningfully parametrized as well as on the discretization of dynamical and physical processes took place so rapidly that it overwhelmed the rare attempts to find consistent sets of equations for intermediate systems.

Part of the basis of the present work is that the third argument is no longer valid, owing to the current stabilization towards the non-hydrostatic compressible Euler equations and prognostic systems for all possible microphysical cloud and precipitation species. Hence it should be no surprise that the subject of a fully consistent set of multiphase dynamical and thermodynamical equations has recently received substantial attention (e.g. Bannon, 2002; Bryan and Fritsch, 2002; Wacker and Herbert, 2003). This happened although the topic could in fact have been addressed already thirty years ago, following for instance some pioneering work of Hinkelmann (developed and published by Zdunkowski and Bott 2003, in chapter 11 of their textbook).

The first constraint for comparing the results of different models is that their diagnostic quantities are unambiguously defined. For this purpose, fluxes have a unique meaning while vertical

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integrals of model tendencies sometimes do not, which draws attention to the importance of the flux-conservative form.

We wish to propose here a set of equations as general and as complete as possible for the rather stable current status of dynamical and physical modelling. The Green–Ostrogradsky theorem, in its vertical one-dimensional form, will be our main reference and target. In doing so we are following fully one of the main conclusions of the benchmarking exercise of Bryan and Fritsch (2002) for moist non-hydrostatic modelling, which notes: '*Both mass-conserving and energy conserving equation sets were required to produce acceptable results.*'. Our aim is also to offer a tool that provides for a formal plug-compatibility rather than a purely technical one. The solution to these challenges may contribute to a set of rules for a common physics–dynamics interface, built around a unique set of equations but adaptable to different modelling contexts. The main result of the present work will indeed be that there exists a rather simple solution satisfying the above ensemble of constraints. Owing to the general character of our starting point and of our rules, this solution should in principle be easily applicable to other frameworks.

Several particular choices are now however necessary for the derivation of this general solution:

– The vertical coordinate is a hybrid terrain-following mass-weighted one, following Simmons and Burridge (1981) for the hydrostatic primitive equations (HPE) system and Laprise (1992) for a non-hydrostatic compressible extension.

– We implicitly restrict the work to the shallow-atmosphere equations, although as shown by Wood and Staniforth (2003) the mass-weighted choice for the vertical coordinate guarantees that it is a fully transparent choice.

– All water species contribute to the mass of the considered 'parcels' and hence precipitating species enter all budget-type computations on an equal footing to other species. As a consequence the velocity of the parcel becomes the full barycentric one.

– Only local forms of the continuity, mass species and thermodynamic equations are considered. The interaction with the vertical momentum and kinetic energy aspects of the problem are not yet treated in this work.

– We assume that the equations automatically obey the Green–Ostrogradsky theorem when turbulent fluxes of enthalpy and water species are derived using Reynolds-type averaging. Wacker and Herbert (2003) indicate that this is a legitimate step when working with a full mass-weighted system.

The starting point of the work described here is the set of simplifying hypotheses of Section 2. The details of the scheme and its framework are described in Section 3. In Section 4, the prognostic equations for the ratios of the different mass species and a basic form of the thermodynamic equation are derived. In Section 5, a full flux-conservative thermodynamic equation is presented for the HPE case. In Section 6, the possibility of projecting the total heat source/sink on both temperature and pressure changes in the compressible case is addressed. Some remarks are given in Section 7 and finally some conclusions are drawn in Section 8.

2. Simplifying hypotheses

The following simplifying hypotheses are made:

– The atmosphere is in permanent thermodynamic equilibrium. This allows the enthalpy budgets to be derived from entropy considerations and flux-divergence forms to be assumed for turbulent- and radiative heat sources/sinks.

– Condensed phases are assumed to have a zero volume. This classical hypothesis allows simplification of the non-compressibility problem for some portion of the atmospheric content.

– All gases (dry air and water vapour) obey Boyle–Mariotte's and Dalton's law. This hypothesis, together with the previous one, allows the state equation for the total parcel content to be written in a tractable form, despite the total-mass approach.

– All specific heat values are independent of temperature. This allows a linear dependence of latent heats upon temperature that nicely commutes with the linear dependence of specific heats upon water contents.

– The temperatures of species inside an elementary portion of the atmospheric mass are assumed to all have the same value for their respective averages. This hypothesis is necessary if one wants to avoid an enormous complexity in the treatment of the thermodynamic budgets once the decision has been made to use a total-mass framework. It is of course less justifiable than the previous hypotheses when considering precipitation species in their falling process (their real temperature is rather the wet-bulb one). But, on the other hand, considering the falling precipitation species 'out of the mass parcel' can lead to even more questionable approximations. A discussion about this problem, considered in more general terms, appears in Sections 5 and 6.

– There is no fictitious counter-flux of dry air to compensate the vertical displacements of water (under all forms). The equations of the present paper can in fact also be written if the (usually implicit) 'compensation' hypothesis is made. A mirror derivation would unnecessarily lengthen the core points of our demonstration and therefore only the final result will be given in Section 7.4.

3. The microphysical scheme

We consider a microphysical scheme with five water species having the following ratios with respect to the total parcel mass: q_v for water vapour, q_l for suspended liquid water, q_r for rain water, q_i for suspended solid water (ice) and q_s for snow. Together with the ratio of dry air, q_d, we have $q_d + q_v + q_l + q_r + q_i + q_s = 1$. The second and third hypotheses of Section 2 imply that one can express the gas constant of the parcel as $R = q_d R_d + q_v R_v$, with R_d and R_v the gas constants of dry air and water vapour.

The suspended water remains in the parcel and only rain water and snow leave the parcel. In a mass-weighted system the associated precipitation fluxes can be written as $P_l = \rho_r w_r$ and $P_i = \rho_s w_s$, where ρ_r and ρ_s are the respective densities of rain water and snow and w_r and w_s their respective vertical fall-speeds with respect to the centre of mass. By convention these fluxes, like every other flux or pseudo flux used in the ensuing developments, are counted positive when directed downwards.

Next to these two mass-weighted fluxes we consider the following pseudo fluxes: P_l' representing the mass-weighted integral of the transfer between water vapour and (suspended) liquid water due to condensation/evaporation; P_l'' idem for the transfer between liquid and rain water due to auto-conversion; P_l''' idem for the transfer between rain water and water vapour due to evaporation of the falling liquid precipitation; P_i' idem for the transfer between water vapour and (suspended) ice due to freezing/sublimation; P_i'' idem for the transfer between ice and snow due to auto-conversion; P_i''' idem for the transfer between snow and water vapour due to sublimation of the falling solid precipitation. Figure 1 gives a schematic representation of the above mentioned (pseudo) fluxes. Section 4.3 will make explicit the link between the various fluxes and pseudo fluxes.

In this way of writing the scheme, only phase changes with respect to water vapour are included: the processes of melting or freezing between solid and liquid phases are therefore considered such that the water goes through the vapour phase. Of course this is physically not the case but thermodynamically it is fully correct. Furthermore all non-precipitating species are assumed to have the same vertical velocity.

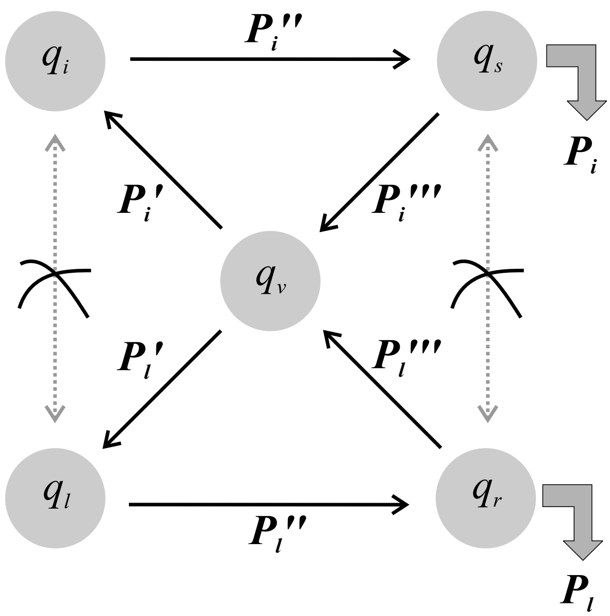

Fig. 1. A schematic representation of the microphysical scheme. All phase-changes go through the vapour phase and only rain and snow leave the parcel. The arrows show the sign convention for the different fluxes in this paper but the exchange between two species can be in both directions.

The use of the full mass-weighted solution for a system where one wishes to keep a 'gaseous-type' state equation may appear counter-intuitive. Nevertheless, Wacker and Herbert (2003) make the same recommendation: '*In a more detailed framework in which the field balance equations of momentum, energy and entropy of the system are also enclosed, a clear physical preference is seen to exist for the barycentric frame of reference.*'. However, they advocate this use of total mass weighting (and necessarily then of the associated barycentric velocity) in a system without falling precipitation species. Considering our proposed extension to such species, there is an analogy with the famous question of the fly under a hermetic cheese-bell on one side of a balanced scale. Whether the fly sits on the bottom or flies at constant level does not change the position of the scale, since it only feels a closed system (bell, bottom, fly and gas). In this case, the gas will indeed not only transmit the pressure forces linked to its independent thermodynamic state but also the compression effect below the wings that allows the fly to stay airborne. Similarly, the total pressure gradient across a given atmospheric layer must take into account the effect of the forces preventing the raindrops from falling with a permanently increasing speed.

In the case when the fly takes off or lands, the situation is a bit different. Indeed, there is no longer a closed system since it is not the centre of mass that will determine the position of the scale but the bottom of the bell. So, when the fly takes off or lands, the bottom of the bell and hence the scale will accelerate. Translating this into a microphysical environment, generation and evaporation of precipitation will induce during a short period in time a change in pressure. The resulting pressure wave will disperse in all directions and eventually also affect the surface pressure.

The way to eliminate any acceleration term for the total mass is to consider a counter-motion by non-precipitating species (or part of them) that leads to additional terms in the relevant equations. Moreover, the compressibility of dry air and water vapour also leads to additional terms. Fortunately, under the simplifying hypotheses described in the above Section, additional terms will cancel out and the resulting set of equations will have the desired flux-conservative property. Thus, a consistent system in which one would decide to neglect one part of the above mentioned acceleration terms through a non-barycentric choice should in principle consider the full complexity of the accelerating phase of the raindrops' fall. This is probably far more cumbersome than the equation system we shall develop in this paper.

The points made in the last two paragraphs are in principle valid only in the case of compressible equations where the diabatic effects on pressure are taken into account (see Section 6). There are two coupled aspects related to this issue: first, the choice of the components entering the continuity equation (dry air, gas, suspended content or total content); second, the dependence on the system of equations (HPE, compressible quasi-anelastic or compressible non-approximated, all as defined in Section 6). We shall assume for the time being that the order in which to address both issues is indifferent.

4. The flux-conservative equations

4.1. At the surface

At the surface, considering an evaporation flux E, a liquid precipitation flux R and a solid precipitation flux S (all positive downwards), one gets the following advective and diffusive fluxes:

Species	Advective	Diffusive
q_d	$g(E+R+S)q_d$	$-g(E+R+S)q_d$
q_v	$g(E+R+S)q_v$	$gE-g(E+R+S)q_v$
q_l	$g(E+R+S)q_l$	$-g(E+R+S)q_l$
q_r	$g(E+R+S)q_r$	$gR-g(E+R+S)q_r$
q_i	$g(E+R+S)q_i$	$-g(E+R+S)q_i$
q_s	$g(E+R+S)q_s$	$gS-g(E+R+S)q_s$

It is readily verified that the sum of all diffusive fluxes is zero. At the surface there exists a total advective flux $g(E+R+S)$ but there is no total flux of q_d, q_l and q_i. There is however no obvious continuity for the diffusive fluxes linked to precipitating species in the atmosphere (in the related equations of Section 4.3 there will be no diffusive fluxes for rain and snow). This discrepancy is in fact a surface–atmosphere interfacing issue that should be treated separately.

4.2. Continuity equation and consequences

Following Simmons and Burridge (1981) and Laprise (1992), one can apply general derivation rules for the total mass-weighted framework. Since there are then no mass fluxes acting as source terms, the continuity equation can be written (in the HPE case, otherwise replace pressure p by hydrostatic pressure π) as

$$\frac{\partial}{\partial t}\left(\frac{\partial p}{\partial \eta}\right) = -\nabla.\left(\vec{v}\frac{\partial p}{\partial \eta}\right) - \frac{\partial}{\partial \eta}\left(\dot{\eta}\frac{\partial p}{\partial \eta}\right), \quad (1)$$

with $\vec{v}$ the horizontal wind vector and η a hybrid pressure-type vertical coordinate. The vertical velocities at the upper and lower boundaries are:

$$\eta = 0 \quad \rightarrow \quad \dot{\eta}\frac{\partial p}{\partial \eta} = 0, \quad (2)$$

$$\eta = 1 \quad \rightarrow \quad \dot{\eta}\frac{\partial p}{\partial \eta} = g(E+R+S). \quad (3)$$

Integrating the above continuity equation over $\eta = 0 \rightarrow 1$ and using the boundary conditions (2) and (3), the surface pressure (p_s) tendency can be written as

$$\frac{\partial p_s}{\partial t} = -\int_0^1 \nabla.\left(\vec{v}\frac{\partial p}{\partial \eta}\right) \mathrm{d}\eta - g(E+R+S). \quad (4)$$

When using the general definition of η, $p(\eta) = A(\eta) + B(\eta)p_s$, a similar derivation as for eq. (10) in Courtier et al. (1991) leads to the following pressure-related vertical velocity:

$$\omega = \vec{v}.\nabla p - \int_0^\eta \nabla.\left(\vec{v}\frac{\partial p}{\partial \eta}\right) d\eta. \quad (5)$$

Here, this expression no longer depends on the precipitation flux, which means that there is no physical forcing needed on ω. This is a first illustration of the strength of the adopted framework.

But here appears a key question which could easily stay unnoticed when superficially considering the final equations which we shall later obtain. When using a mass-weighted framework an asymmetry emerges. Rain droplets and snow flakes cannot compress during their descent to the surface. But dry air and water vapour experience a compensating lift with respect to the centre of mass and these species can then expand.

We shall now translate this into a mathematical expression. One may define two different frameworks: (1) a fixed one which works with the gaseous species and (2) a full mass-weighted one which treats all species. The transition between these two frameworks can be expressed as follows:

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{\mathrm{all}} = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{\mathrm{gas}} + g(P_l+P_i)^*\frac{\partial}{\partial p} \quad (6)$$

with $(P_l + P_i)^*$ the absolute precipitation fluxes (see Section 7.2 for the conversion from relative to absolute fluxes). Consequently, one finds

$$\omega_{\mathrm{all}} = \omega_{\mathrm{gas}} + g(P_l+P_i)^*. \quad (7)$$

In the following, we shall continue working in the full mass-weighted system.

4.3. Prognostic equations for the different species

In the mass-weighted framework the precipitation fluxes will cause a compensating lift (referred to the centre of mass) of all non-precipitating species (dry air, water vapour, suspended liquid and solid water). The corresponding fluxes of these species should cancel out the total precipitating flux. Hence we can write this compensating flux for e.g. the water vapour part (and similarly for the other non-precipitating species) as

$$\frac{q_v(P_l+P_i)}{q_d+q_v+q_l+q_i} = \frac{q_v(P_l+P_i)}{1-q_r-q_s}. \quad (8)$$

The conservation of water vapour can then be expressed as

$$\frac{\partial}{\partial t}\left(q_v \frac{\partial p}{\partial \eta}\right) = -\nabla.\left(q_v \vec{v} \frac{\partial p}{\partial \eta}\right) - \frac{\partial}{\partial \eta}\left(q_v \dot{\eta} \frac{\partial p}{\partial \eta}\right) - g\frac{\partial}{\partial \eta}\left(P_l' - P_l''' + P_i' - P_i''' - \frac{q_v(P_l + P_i)}{1 - q_r - q_s}\right) - g\frac{\partial J_{q_v}}{\partial \eta}, \tag{9}$$

with J_{q_v} the turbulent flux of water vapour. Subtracting q_v times the continuity equation and multiplying by $\partial\eta/\partial p$ gives the following physical tendency

$$\frac{\mathrm{d}q_v}{\mathrm{d}t} = g\frac{\partial}{\partial p}\left[P_l''' + P_i''' - P_l' - P_i' + \frac{q_v(P_l + P_i)}{1 - q_r - q_s} - J_{q_v}\right]. \tag{10}$$

Similarly one obtains

$$\frac{\mathrm{d}q_l}{\mathrm{d}t} = g\frac{\partial}{\partial p}\left[P_l' - P_l'' + \frac{q_l(P_l + P_i)}{1 - q_r - q_s} - J_{q_l}\right] \tag{11}$$

$$\frac{\mathrm{d}q_r}{\mathrm{d}t} = g\frac{\partial}{\partial p}\left[P_l'' - P_l''' - P_l\right] \tag{12}$$

$$\frac{\mathrm{d}q_i}{\mathrm{d}t} = g\frac{\partial}{\partial p}\left[P_i' - P_i'' + \frac{q_i(P_l + P_i)}{1 - q_r - q_s} - J_{q_i}\right] \tag{13}$$

$$\frac{\mathrm{d}q_s}{\mathrm{d}t} = g\frac{\partial}{\partial p}\left[P_i'' - P_i''' - P_i\right] \tag{14}$$

$$\frac{\mathrm{d}q_d}{\mathrm{d}t} = g\frac{\partial}{\partial p}\left[\frac{q_d(P_l + P_i)}{1 - q_r - q_s} - J_{q_d}\right], \tag{15}$$

where J_{q_l}, J_{q_i} and J_{q_d} are the turbulent fluxes of the respective species, with $J_{q_d}+J_{q_v}+J_{q_l}+J_{q_i}=0$. This ensures that all terms on the right hand sides cancel out.

4.4. *The thermodynamic equation*

The derivation of the thermodynamic equation starts with the general entropy (S) expression given by Marquet (1993) (who extended the work of Hauf and Höller, 1987) which we multiply by q_d in order to have an expression per unit of mass:

$$S' = q_d S = (q_d c_{pd} + q_t c_{pv})\ln\frac{T}{T^*} - q_d R_d \ln\frac{(p-e)}{(p-e)^*} - q_t\left(R_v \ln\frac{e}{e^*} - \frac{L_i^*}{T^*}\right) - \frac{L_l(T)}{T}(q_l + q_r) - \frac{L_i(T)}{T}(q_i + q_s), \tag{16}$$

where S' is the total entropy per unit of mass, $q_t = q_v + q_l + q_r + q_i + q_s$ corresponds to the total water substance, $T^* = 0°\mathrm{C}$ is the reference temperature, $(p - e)^* = 10^5$ Pa the reference dry air pressure, $e^* = 610.7$ Pa the reference saturation vapour pressure (at 0°C), $L_l(T)$ the latent heat change for liquid water, $L_i(T)$ the latent heat change for solid water and L_i^* the reference latent heat for sublimation at 0°C. Note that this expression is valid for a closed system and hence does not include transport processes which will be considered below.

The time-derivative of S' will therefore be the change in entropy due to external processes (such as radiation, turbulence and precipitation) which will be represented by the external diabatic heat source $\widetilde{Q}$. From this heat source we can subtract the changes in entropy due to changes in the mass of species associated with both turbulent and precipitation related fluxes. Note that both these effects have, although on different scales, a diffusive character: the precipitation related fluxes actually represent the deviations from the barycentric flow and are hence 'organized' (i.e. resolved by the model), while the truly diffusive turbulent fluxes are supposed to be homogeneous and of course unresolved.

Subtracting these two effects actually means that $\widetilde{Q}$ will be replaced by a new heat source $\overline{Q}$ out of which both effects are filtered. The remaining contributions to $\overline{Q}$ are the divergences of the thermodynamic diffusive flux J_s and of the radiative flux J_{rad}. The change in entropy due to turbulence can be expressed as

$$-g\left(c_{pd}\frac{\partial J_{q_d}}{\partial p} + c_{pv}\frac{\partial J_{q_v}}{\partial p} + c_l\frac{\partial J_{q_l}}{\partial p} + c_i\frac{\partial J_{q_i}}{\partial p}\right). \tag{17}$$

The change in entropy due to precipitation can be written as a sum of entropy-fluxes associated with the different precipitation-related mass-fluxes which appeared in eqs. (10)–(15). The entropy of each species can be defined similarly as in Bannon (2002), cf. his eqs. (7.11)–(7.15). Following all the above steps, we finally find

$$\overline{Q} = c_p\frac{\mathrm{d}T}{\mathrm{d}t} - \frac{1}{\rho}\frac{\mathrm{d}p}{\mathrm{d}t} - gL_l(T)\frac{\partial}{\partial p}(P_l' - P_l''') - gL_i(T)\frac{\partial}{\partial p}(P_i' - P_i''') + g\frac{P_l + P_i}{\rho(1 - q_r - q_s)} + g\left[c_l P_l + c_i P_i - \frac{c_p - c_l q_r - c_i q_s}{1 - q_r - q_s}(P_l + P_i)\right]\frac{\partial T}{\partial p} - gT\left(c_{pd}\frac{\partial J_{q_d}}{\partial p} + c_{pv}\frac{\partial J_{q_v}}{\partial p} + c_l\frac{\partial J_{q_l}}{\partial p} + c_i\frac{\partial J_{q_i}}{\partial p}\right) \tag{18}$$

with c_p the total specific heat at constant pressure of the parcel, obtained by a linear combination of the specific heat values of the species, weighted by their respective mass contributions.

Equation (18) is derived for the full system, i.e. both dynamics and physics are treated simultaneously. The pure physical processes that influence the thermodynamical properties of a parcel are precipitation, phase-changes, radiation and turbulent fluxes. Due to the compensating lift of the non-precipitating species, compensating enthalpy fluxes will appear in the mass-weighted environment. Hence the total diabatic heat source can be written as

$$Q = \overline{Q} + gL_l(T)\frac{\partial}{\partial p}(P_l' - P_l''') + gL_i(T)\frac{\partial}{\partial p}(P_i' - P_i''') - g\left[c_l P_l + c_i P_i - \frac{c_p - c_l q_r - c_i q_s}{1 - q_r - q_s}(P_l + P_i)\right]\frac{\partial T}{\partial p} + gT\left(c_{pd}\frac{\partial J_{q_d}}{\partial p} + c_{pv}\frac{\partial J_{q_v}}{\partial p} + c_l\frac{\partial J_{q_l}}{\partial p} + c_i\frac{\partial J_{q_i}}{\partial p}\right). \quad (19)$$

Using the expression above, (18) can be put in a more classical form:

$$c_p\frac{\mathrm{d}T}{\mathrm{d}t} - RT\frac{\mathrm{d}\ln(p)}{\mathrm{d}t} + g\frac{1}{\rho}(P_l + P_i)^* = Q. \quad (20)$$

This expression was derived without any reference to whether one uses HPE or compressible conditions and is in fact a variant of the well known version of the thermodynamic equation. The (additional) third term, which expresses in fact the dynamical impact of the formation or evaporation of precipitation, will appear only when the acceleration due to precipitation is not countered by something. We will develop in the next two Sections two sets of equations which reflect the truth of the steady state (i.e. where the additional dynamical impact is filtered out) with only a minimum of approximations. This calls for treating together the thermodynamics and dynamics of the system.

5. Final equations under the hydrostatic conditions

In Section 3, we noted that the formation and evaporation of precipitation has a dynamical impact and this impact indeed appears in the thermodynamic eq. (20). In the HPE case however, the hydrostatic approximation filters out the adjustment pressure waves caused by the formed or evaporated precipitation. This means that in this case the acceleration $g(P_l + P_i)^*/\rho$ is automatically compensated for. In this spirit we rewrite (20) as

$$c_p\frac{\mathrm{d}T}{\mathrm{d}t} - RT\frac{\mathrm{d}\ln(p)}{\mathrm{d}t} = Q' \quad (21)$$

with $Q' = Q - g(P_l + P_i)^*/\rho$ the diabatic heat source out of which the additional dynamical acceleration is filtered. This quantity can also be expressed as the following temperature tendency:

$$c_p\frac{\partial T}{\partial t} = gL_l(T)\frac{\partial}{\partial p}(P_l' - P_l''') + gL_i(T)\frac{\partial}{\partial p}(P_i' - P_i''') - g\left[c_l P_l + c_i P_i - \frac{c_p - c_l q_r - c_i q_s}{1 - q_r - q_s}(P_l + P_i)\right]\frac{\partial T}{\partial p} - g\frac{\partial J_s}{\partial p} + gT\left(c_{pd}\frac{\partial J_{q_d}}{\partial p} + c_{pv}\frac{\partial J_{q_v}}{\partial p} + c_l\frac{\partial J_{q_l}}{\partial p} + c_i\frac{\partial J_{q_i}}{\partial p}\right) - g\frac{\partial J_{\mathrm{rad}}}{\partial p}, \quad (22)$$

where we used on the left hand side the partial time derivative to stress that we now only treat the physical tendency. Writing c_p as $c_p = c_{pd}q_d + c_{pv}q_v + c_l(q_l + q_r) + c_i(q_i + q_s)$ and using $L_{l|i}(T) = L_{l|i}(T_0) + (c_{pv} - c_{l|i})T$ with $T_0 = 0\ K$, (22) can be rewritten by expressing the physical tendency of the enthalpy c_pT instead of the temperature T, or

$$\frac{\partial}{\partial t}(c_pT) = -g\frac{\partial}{\partial p}\big[(c_l - c_{pd})P_lT + (c_i - c_{pd})P_iT - (\hat{c} - c_{pd})(P_l + P_i)T + J_s + J_{\mathrm{rad}} - L_l(T_0)(P_l' - P_l''') - L_i(T_0)(P_i' - P_i''')\big], \quad (23)$$

where

$$\hat{c} = \frac{c_{pd}q_d + c_{pv}q_v + c_lq_l + c_iq_i}{1 - q_r - q_s}. \quad (24)$$

The terms on the right hand side of (23) which represent the enthalpy changes due to precipitation result from (a) an impact of the $L_{l|i}(T)$ dependency, (b) 'real' enthalpy transport by the different species and (c) enthalpy transport by the compensating lift fluxes of the non-precipitating species.

The sum of contributions (b) and (c) represents, for the precipitation process, the type of residual which Bannon (2002) claims can be ignored (cf. his eq. 6.3 and the ensuing sentences). However, order of magnitude computations of this term lead to surface balance impacts of the order of a few W/m^2. And even if it would not be the case, let us recall another conclusion of the work of Bryan and Fritsch (2002): '*The neglect of one typically small term from the thermodynamic equation unexpectedly produced the worst results, highlighting the danger of using scale analysis to neglect terms from the governing equations.*'. Furthermore, thanks to the mass-weighted environment, the whole right hand side of (23) can be written as the true divergence of a sum of fluxes. In short

$$\frac{\partial}{\partial t}(c_pT) = -g\frac{\partial J_{\mathrm{total}}}{\partial p} \quad (25)$$

with J_{total} a short-hand simplifying notation indicating that (23) truly obeys the Green–Ostrogradsky rule.

Comparison of (25) and (21) gives an alternative expression for Q':

$$Q' = -g\frac{\partial J_{\mathrm{total}}}{\partial p} - T\frac{\mathrm{d}c_p}{\mathrm{d}t}, \quad (26)$$

so that (21) takes the following flux-conservative form:

$$\frac{\mathrm{d}(c_pT)}{\mathrm{d}t} - RT\frac{\mathrm{d}\ln(p)}{\mathrm{d}t} = -g\frac{\partial J_{\mathrm{total}}}{\partial p}. \quad (27)$$

6. Heat source/sink projection on temperature and pressure changes

The above is true only when the addition/removal of heat is projected solely on a temperature change and has no pressure change equivalent. This is of course not a problem in the hydrostatic case where the continuity equation is actually a diagnostic relation:

$$\frac{\mathrm{d}\ln(\rho)}{\mathrm{d}t} + D_3 = 0 \quad \text{or} \quad c_v\frac{\mathrm{d}\ln(p)}{\mathrm{d}t} + c_pD_3 = 0, \quad (28)$$

with D_3 the three-dimensional divergence. When leaving the hydrostatic case and using the compressible (or fully elastic) mode, Laprise (1998) and Thurre and Laprise (1996) show that the continuity equation should ideally be expanded to include a thermodynamic forcing (going from their 'quasi-anelastic' case to their 'non-approximated' one). Following (7), the general thermodynamic eq. (20) can be expressed as

$$c_p \frac{\mathrm{d}T}{\mathrm{d}t} - \frac{p_{\text{gas}}}{\rho} \frac{\mathrm{d}\ln p_{\text{gas}}}{\mathrm{d}t} = Q \tag{29}$$

with $p_{\text{gas}} = \rho_{\text{gas}} R_{\text{gas}} T$, where $\rho_{\text{gas}} = \rho_d + \rho_v$ is the density of dry air plus water vapour and R_{gas} the associated gas constant. Put differently,

$$R_{\text{gas}} = \frac{1}{\rho_d + \rho_v}(\rho_d R_d + \rho_v R_v) = \frac{\rho}{\rho_{\text{gas}}} R. \tag{30}$$

Expanding p_{gas} and R_{gas} and using $p_{\text{gas}}/\rho = \rho_{\text{gas}} R_{\text{gas}} T/\rho = RT$, (29) becomes

$$c_p \frac{\mathrm{d}T}{\mathrm{d}t} - RT\frac{\mathrm{d}\ln R}{\mathrm{d}t} - RT\frac{\mathrm{d}\ln \rho}{\mathrm{d}t} - RT\frac{\mathrm{d}\ln T}{\mathrm{d}t} = Q \tag{31}$$

or

$$c_v \frac{\mathrm{d}T}{\mathrm{d}t} + RT D_3 = Q + T\frac{\mathrm{d}R}{\mathrm{d}t}. \tag{32}$$

When doing the inverse calculation, one would exactly find back

$$c_p \frac{\mathrm{d}T}{\mathrm{d}t} - RT\frac{\mathrm{d}\ln(p)}{\mathrm{d}t} = Q. \tag{33}$$

This tells us that identifying, through $p = \rho_{\text{gas}} R_{\text{gas}} T$, the pressure field by the pressure of gases (and hence ignoring any impact of condensates on the stress vector) in fact filters out the change in internal energy due to the change of kinetic energy of the vertically moving species. The equivalent in the previous Section was the usage of the hydrostatic approximation. Hence, similarly to the HPE case, this means that Q can be replaced by Q' in any form of the thermodynamic equation:

$$c_p \frac{\mathrm{d}T}{\mathrm{d}t} - RT\frac{\mathrm{d}\ln(p)}{\mathrm{d}t} = Q'. \tag{34}$$

Equation (34) will allow us to write also in the compressible case a full conservative system of equations. Indeed, using the time derivative of the logarithmic form of the state law and the still valid relationship $c_p = c_v + R$, (34) leads to

$$c_v \frac{\mathrm{d}\ln(p)}{\mathrm{d}t} + c_p D_3 = \frac{Q'}{T} + \frac{c_p}{R}\frac{\mathrm{d}R}{\mathrm{d}t}. \tag{35}$$

To summarize, one uses in the filtered (hydrostatic and anelastic) cases the set of equations formed by (21) and (28), whereas in the compressible case one has the option to use the set formed by (34) and (35). Better said, when returning to a flux-conservative form in the compressible framework, one can choose between the quasi-anelastic solution

$$\frac{\mathrm{d}(c_p T)}{\mathrm{d}t} - RT\frac{\mathrm{d}\ln(p)}{\mathrm{d}t} = -g\frac{\partial J_{\text{total}}}{\partial \pi} \tag{36}$$

$$\frac{\mathrm{d}\ln(p)}{\mathrm{d}t} + \frac{c_p}{c_v} D_3 = 0 \tag{37}$$

and the more advanced non-approximated solution (rearranging 34 and 35)

$$\frac{\mathrm{d}(c_v T)}{\mathrm{d}t} + RT D_3 = -g\frac{\partial J_{\text{total}}}{\partial \pi} \tag{38}$$

$$\frac{\mathrm{d}\ln(c_v p/R)}{\mathrm{d}t} + \frac{c_p}{c_v} D_3 = -\frac{g}{c_v T}\frac{\partial J_{\text{total}}}{\partial \pi}. \tag{39}$$

For 'filtered' cases (37) disappears and p replaces π in (36). These various sets are always complemented by eqs. (10)–(15).

7. Some remarks

7.1. Linking the hydrostatic and compressible cases

We demonstrated in the two previous Sections that one can filter out the additional dynamical term (as mentioned at the end of Section 4.4) for both the HPE and compressible case. The central link between the thermodynamics and dynamics used in the filtering process is in fact the equivalence of the state equation ($p = \rho_{\text{gas}} R_{\text{gas}} T = \rho RT$). The mathematical demonstration is easier in the compressible case but it offers an a posteriori justification for the more intuitive application in the HPE case (where $dp = -\rho g dz$ mixes the specific filtering with other considerations).

7.2. Absolute versus relative motions

If we define as $P_l^* = w_r^* \rho_r$ and $P_i^* = w_s^* \rho_s$ the respective rain and snow fluxes as seen by a given microphysical computation (the 'absolute' fluxes, with w_r^* and w_s^* the 'absolute' falling speeds), then the corresponding fluxes with respect to the centre of mass can be expressed as

$$P_l = w_r \rho_r = (1 - q_r) P_l^* - q_r P_i^* \tag{40}$$

$$P_i = w_s \rho_s = (1 - q_s) P_i^* - q_s P_l^*, \tag{41}$$

so that

$$P_l + P_i = (1 - q_r - q_s)(P_l + P_i)^*. \tag{42}$$

One may then rearrange all previous equations in terms of absolute fluxes.

7.3. Infinite fall-speed for precipitating species

A practice sometimes applied in large scale Numerical Weather Prediction (NWP) is to remove the generated precipitation within one time-step. Two hypotheses can help simulating this here: (1) the mass of precipitation is neglected ($q_r = q_s = 0$) and (2) the assumed fall-speed of the precipitating species has an infinite value ($w_r = w_s = \infty$). Since in this case one assumes that the

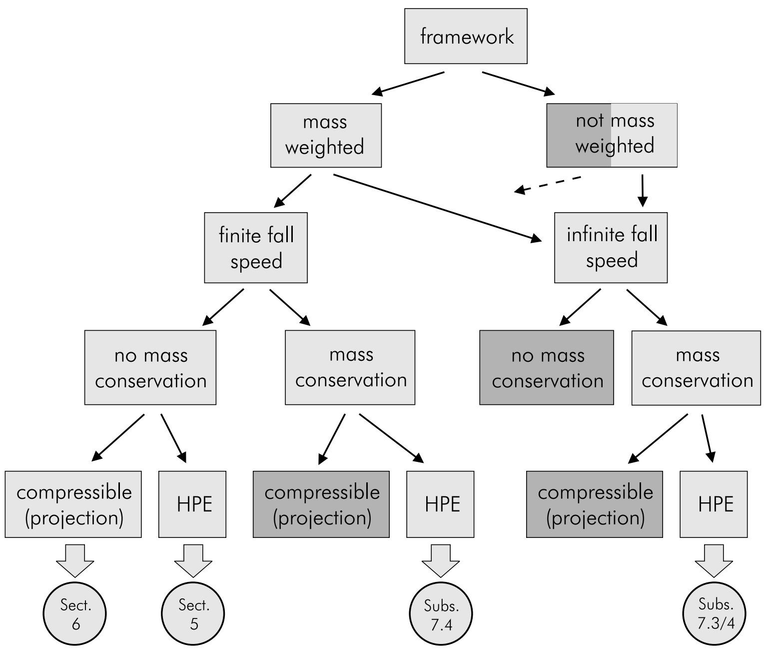

Fig. 2. A visualization of the many options and possible combinations which were treated in this paper. The rectangles in dark grey correspond to unrecommended choices. The advocated solutions are in increasing order of realism when going from right to left.

precipitation flux has a finite value ($P = \infty \times 0$), it is easily verified that when using the above two conditions, the equations derived in the present paper are still valid.

7.4. *Fictitious counter-flux of dry air*

A hypothesis frequently made in NWP is that any mass flux due to the motion of moisture is compensated by a counter-flux of dry air. This is equivalent to having an unchanged continuity equation with respect to the adiabatic case and is thus often done by default rather than on purpose. In the present case the centre of mass does not have a vertical velocity so there is no longer a need for a compensating lift of non-precipitating water species. Hence counter-fluxes of the type of (8) will disappear in the prognostic equations, which also eliminates the term $(\hat{c} - c_{pd})(P_l + P_i)T$ in the thermodynamic equation. The equations describing the conservation of the species are consequently similar to eqs. (10)–(15) but without the terms with $(1 - q_r - q_s)$ as denominator. The full thermodynamic equation can then be expressed as

$$\frac{\mathrm{d}(c_p T)}{\mathrm{d}t} - RT\frac{\mathrm{d}\ln(p)}{\mathrm{d}t} + g\frac{1}{\rho}(P_l + P_i)^* \frac{\partial(p-e)}{\partial p} = -g\frac{\partial J'_{\text{total}}}{\partial p} \tag{43}$$

with J'_{total} the equivalent of J_{total} determined by the following expression

$$-g\frac{\partial J'_{\text{total}}}{\partial p} = -g\frac{\partial}{\partial p}\Big[(c_l - c_{pd})P_l T + (c_i - c_{pd})P_i T + J_s + J_{\text{rad}} - L_l(T_0)(P'_l - P'''_l) - L_i(T_0)(P'_i - P'''_i)\Big]. \tag{44}$$

Again a term due to vertically moving species appears, although now only linked to dry air. A development similar to that in Section 5 allows us to remove this term and the resulting thermodynamic equation is the same as (27) where J_{total} is replaced by J'_{total}.

This new set of equations is simpler than the one developed in the core of the present paper, but it is less exact, even if probably more suitable in the reduced framework of Section 7.3.

7.5. *Portability*

In the three previous subsections, we demonstrated the flexibility of the core development. As illustration, Figure 2 displays a decision tree indicating the possibilities alluded to in the text. Further, it should be possible to extend the sets of equations obtained here to other frameworks, for instance with different vertical coordinate systems. The main reason for this flexibility is the consistent use of a total mass-weighted framework.

8. Conclusions

There exists an exact flux-conservative form of all thermodynamic-type equations even when taking into account all relevant heat sources/sinks and accounting for all important prognostic aspects of complex cloud- and precipitation processes. The key to this result lies in: (1) the choice of complementary basic hypotheses (letting for instance both L vary with T and c_p vary with q_x), (2) a minimal approximation for the transition from the non-precipitating to the precipitating case or vice-versa and (3) the consistent use of a total-mass based ('barycentric') system. The latter point is even emphasized when extending the results, still in a flux-conservative form, from the 'classical' HPE case to the compressible case, a step made possible here by the use of the hydrostatic pressure vertical coordinate of Laprise (1992).

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