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On the definition of a moist-air potential vorticity.

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Abstract

A new potential vorticity is derived by using a specific entropy formulation expressed in terms of a moist-air entropy potential temperature. The new formulation is compared with Ertel's version and with others based on virtual and equivalent potential temperatures. The new potential vorticity is subject to conservative properties ensured by the Second Law applied to the moist-air material derivatives. It is shown that the upper tropospheric and stratospheric (dry) structures are nearly the same as those obtained with Ertel's component. Moreover, new structures are observed in the low troposphere, with negative values associated with moist frontal regions. The negative values are observed in the frontal regions where slantwise convection instabilities may take place, but they are smaller than those observed with the equivalent potential vorticity. The main purpose of the article is to diagnose the behaviour of the new potential vorticity from numerical output generated by the ARPEGE NWP model, with the help of isobaric charts and vertical cross-sections. Two inversion methods are suggested. The first method could be based on the invertibility principle verified by the virtual potential vorticity, with a possibility to control and modify separately potential vorticity components in the (dry) upper and (moist) lower atmospheric levels. The other method may consist of an inversion process directly applied to the new moist-air entropy potential vorticity, because the negative values and the solenoidal term are smaller than those observed with equivalent potential vorticity, as shown by numerical evaluations.

1 Introduction.

The aim of the present article is to extend the definition of the moist version of the potential vorticity defined in Schubert *et al.* (2001, hereafter referred to as S01), by taking into account the moist entropy formulation derived in Marquet (2011, hereafter referred to as M11).

With the notation introduced in Appendix A and according to Hoskins *et al.* (1985, hereafter referred to as H85), the potential vorticity function of any real variable ψ may be defined by

$$PV(\psi) = \frac{1}{\rho} \zeta_a \cdot \nabla(\psi). \quad (1)$$

It depends on the density ρ and the absolute vorticity $\zeta_a = 2\boldsymbol{\Omega} + \nabla \times \mathbf{u}$. The corresponding *PV* equation, valid for a hydrostatic atmosphere and for any scalar variable ψ , is written as

$$\rho \frac{d}{dt} [PV(\psi)] = \frac{1}{\rho^2} \nabla(\psi) \cdot [\nabla(\rho) \times \nabla(p)] + \zeta_a \cdot \nabla \left(\frac{d\psi}{dt} \right) + (\nabla \times \mathbf{F}) \cdot \nabla(\psi). \quad (2)$$

It is mentioned in H85 that “Normally in meteorology, ψ is taken to be the potential temperature, although it can be equally well be taken to be the specific entropy or any other function of potential

temperature'. The original Ertel formulation (1942, English translations in Schubert *et al.*, 2004) indeed corresponds to the case $\psi = \theta$, where the dry-air potential temperature is equal to

$$\theta = T \left(\frac{p_0}{p} \right)^\kappa . \quad (3)$$

The *PV* thinking popularized by H85 makes use of this formulation which demonstrates at the same time a Lagrangian conservation property and a principle of invertibility for adiabatic, reversible and frictionless motion of dry air.

The reason why the choice of $\psi = \theta$ annihilates the solenoidal term in the first line of the R.H.S. of (2) is that θ can be expressed in terms of ρ and p only, according to the dry-air equation of state which may be written

$$p = \rho R_d T = \rho R_d \theta \left(\frac{p}{p_0} \right)^\kappa , \quad (4)$$

$$\theta(\rho, p) = \frac{p}{\rho R_d} \left(\frac{p_0}{p} \right)^\kappa . \quad (5)$$

The second line in the R.H.S. of (2) also cancels out for the adiabatic, reversible and frictionless motion of dry air, because the first term depends on the material derivative of θ and is equal to zero since the dry-air entropy $s = c_{pd} \ln(\theta) + C^{ste}$ corresponds to the property $d\theta/dt = (\theta/c_{pd}) ds/dt = 0$. The last term of (2) depends on the curl of the friction force and it vanishes for frictionless motion. As a consequence, the material derivative (2) is indeed equal to zero for $\psi = \theta$ and during the reversible, adiabatic and frictionless motion of a parcel of dry air.

Ertel's formulation is often used to study the thermodynamical properties of moist atmosphere, though it is based on θ and not on a moist counterpart. It is assumed that the impact of water phase change can be represented by the diabatic term $d\theta/dt$ (i.e. condensation-evaporation and radiative processes). However, the corresponding inversion method does not generate tendencies for water species and the anomalies of $PV(\theta)$ are of small amplitude in the lower troposphere, creating difficulties for (or even an impossibility of) the analysis of the signals associated with frontal or convective moist systems.

In order to avoid these drawbacks, moist versions of the potential vorticity have been used in studies of atmospheric systems. Various moist formulations of *PV* have been built and tested by following the advice of H85, with ψ replaced by the wet bulb (θ'_w), moist entropic (θ_S), equivalent (θ_e), saturation equivalent (θ_{es}) or virtual (θ_v) potential temperatures.

Bennetts and Hoskins (1979, hereafter referred to as BH79) and Emanuel (1979, 1983) have investigated the generation of conditional symmetric instability in baroclinic systems as a possible mechanism for the formation of frontal rain-bands. It is suggested that negative moist potential vorticity computed with either $\psi = \theta'_w$, θ_e or θ_{es} is a sufficient condition for two-dimensional frictionless conditional symmetric instability. However, none of these potential temperatures fulfills the demand to verify, at the same time, a moist conservative property and an invertibility principle.

More precisely, it is shown in S01 and Schubert (2004, hereafter referred to as S04) that, even if the equivalent potential temperatures θ_e or θ_{es} are approximately conserved during the motions of parcels of moist saturated air, and as far as the moist entropy may indeed be approximated by $c_{pd} \ln(\theta_e)$ or $c_{pd} \ln(\theta_{es})$, the solenoidal term in the first line of the R.H.S. of (2) does not cancel out. This is an cumbersome source/sink term which cannot be associated with any conservative law. Moreover, $PV(\theta_e)$ do not verify an invertibility principle.

In a symmetric way, it is shown in S01 and S04 that the choice of the virtual potential temperature $\psi = \theta_v$ annihilates the solenoidal term in (2) and that $PV(\theta_v)$ demonstrates an invertibility principle. However, the corresponding diabatic term $d\theta_v/dt$ does not receive a clear physical

interpretation, since it does not correspond to any moist conservative law. In fact, θ_v is the key quantity used for buoyancy analyses, but it cannot be related to the moist entropy or to the Second Law, or to the conservation of matter for the mixing of dry air and total water species.

It is mentioned in Davies and Wernli (1997) that the PV perspective is founded in three notions:

- i) PV conservation in the adiabatic and frictionless limit;
- ii) PV inversion in the balance-flow limit to obtain the associated flow and thermal pattern;
- iii) PV partition of the field into coherent distinctive elements of potential vorticity and potential temperature. The aim of the present paper is to explore mainly the third notion.

The article is organized as follows. Existing moist potential vorticities are described in Section 2. The main properties of the specific moist entropy, computed in M11 in terms of θ_s , are described in Section 3. The new moist potential vorticity PV_s is defined in Section 4, together with the virtual component PV_v and with the justification for the use of a corresponding new potential vorticity unit (PVUS). An approximate formulation for PV_s is derived in Appendix B, which uses the approximation of θ_s by $(\theta_s)_1$ described in M11. The numerical experimentation is introduced in Section 5, where some isobaric and iso- PV charts are shown. The cross-sections of potential temperatures are presented in Section 6. Isobaric charts and cross-sections of the new potential vorticity components are depicted in Section 7 and 8, respectively. The possibility that the paradigm of slantwise convection may be revisited by the use of PV_s and θ_s is analyzed in Section 9. Charts of low-levels potential vorticity are shown in Section 10 for a large northern midlatitudes Atlantic domain and for two successive forecasts. Hints for next inversion methods based on the use of PV_s are described in Section 11 and in Appendices C and D, for both non-saturated and saturated moist air. Use of new water component is suggested defined by $PV_q = PV_s - PV_v$ which highlight the negative lower-level PV signals associated with moist processes. It is explained that the magnitude of negative values and of solenoidal terms are smaller with the use of θ_s than with the use of θ_e , two interesting features which could motivate a revival of interest in the search for a moist-air inversion tool applied directly to PV_s . Finally, conclusions and outlines are presented in Section 12.

2 Existing moist potential vorticities.

The possibility of defining moist generalizations of Ertel’s potential vorticity has been investigated by many authors.

The wet bulb potential temperature was used in BH79 to define the potential vorticity as

$$q_w = f \frac{g \rho}{\theta_0} PV(\theta'_w). \quad (6)$$

In fact, θ'_w is conserved only during pseudo-adiabatic ascents of a saturated and precipitating convective parcel. The conservative property verified by θ'_w corresponds to irreversible processes of open systems, during which the condensed water is continuously removed from the parcels, resulting in the non-conservation of the moist entropy (a part of which is withdrawn by the precipitations).

Rivas Soriano and García Díez (1997) replaced θ'_w by the entropic potential temperature defined in Hauf and Höller (1987), in order to take into account the impact of ice water. The resulting potential vorticity is written as

$$q_g = f \frac{g \rho}{\theta_0} PV(\theta_S), \quad (7)$$

where the specific moist entropy is defined by $q_d s_r^* + q_d c_p^* \ln(\theta_S/T_0)$. The drawback of this formulation is that the terms s_r^* and c_p^* both depend on r_t , and thus vary with the total water mixing

ratio. The consequence is that the entropic potential temperature θ_S is not trully synonymous with the moist entropy, and q_g cannot establish a general Second-Law conservative property (see M11).

In geostrophic coordinates, the moist potential vorticity is defined in Emanuel *et al.* (1987) with the saturation moist entropy s_e expressed by $c_{pd} \ln(\theta_{es})$, where the equivalent potential vorticity is written in terms of this saturation equivalent potential temperature θ_{es} , leading to

$$q_{ge} = \frac{g \rho}{f \theta_e} PV(\theta_{es}), \quad (8)$$

$$\theta_{es} \approx \theta \exp \left[- \frac{L_{vap} r_{sw}}{c_{pd} T} \right]. \quad (9)$$

The moist generalizations $PV(\theta_v)$ and $PV(\theta_e)$ are tested in S01, where the virtual potential temperature is defined by

$$\theta_v = \theta (1 + \delta q_v - q_l - q_i), \quad (10)$$

and the equivalent potential temperature by

$$\theta_e = T_0 \exp(s_e/c_{pd}). \quad (11)$$

The equivalent entropy s_e appearing in (11) is determined according to Emanuel (1994). It is expressed by two different formulas, depending on saturation or non-saturation conditions.

The moist-air equation of state is expressed in S01 in terms of the virtual potential temperature, leading to

$$p = \rho R_d \theta_v \left(\frac{p}{p_0} \right)^\kappa, \quad (12)$$

$$\theta_v(\rho, p) = \frac{p}{\rho R_d} \left(\frac{p_0}{p} \right)^\kappa. \quad (13)$$

The important property described in S01 is that θ_v given by (13) only depends on ρ and p , as in (5) for the dry-air formulation θ . As a consequence the solenoidal term cancels out in (2) for $\psi = \theta_v$. The corresponding moist PV is defined in S01 by

$$PV(\theta_v) = \frac{1}{\rho} \zeta_a \cdot \nabla(\theta_v). \quad (14)$$

It is then demonstrated in S01 and S04 that $PV(\theta_v)$ follows an invertibility principle, indicating that the virtual potential temperature may be a good candidate to build a moist version for the potential vorticity. However, the main drawback of the choice of $\psi = \theta_v$ is that the material derivative of θ_v does not correspond to a conservative property. Indeed, the gradient of $d\theta_v/dt$ cannot be linked to the change in moist entropy, or to the conservation of dry air and water species, for instance. As a result, the second line in the R.H.S. of the PV equation (2) does not cancel out for $\psi = \theta_v$.

It is suggested in S01 and S04 that it is possible to overcome this drawback by defining the moist PV equation (2) with $\psi = \theta_e$ or θ_{es} . Indeed, the material derivative $d\theta_e/dt$ or $d\theta_{es}/dt$ could be equal to zero for two different reasons.

This might be true for adiabatic and reversible processes if θ_e or θ_{es} were valid measurements of the moist air entropy. This assumption is made for instance in Emanuel *et al.* (1987), with a moist entropy implicitly defined by

$$s = q_d s_e = q_d c_{pd} \ln(\theta_e) + q_t C_1 + q_t C_2. \quad (15)$$

The two terms C_1 and C_2 represent additional terms which are either constant or depends on q_t , with q_t also assumed to be a constant conservative quantity.

However, neither θ_e nor θ_{es} are valid measurements of the more general moist-air specific entropy, as shown in M11. The main problem is that q_d and q_t are located outside the logarithm of θ_e in (15) and that a source of variability due to $q_d = 1 - q_t$ is thus missing in θ_e . Another impact of varying q_d and q_t in (15) is that $q_d C_1$ and $q_t C_2$ become variable terms which cannot be neglected, even if C_1 or C_2 were true constant terms. Moreover, c_{pd} is replaced by $c_{pd} + r_t c_l$ in Emanuel (1994), with the impact of $r_t c_l$ also missing in θ_e .

The facts that θ_e or θ_{es} are considered as conserved quantities, and that the material derivatives are almost equal to zero, correspond to pseudo-adiabatic conservative properties which are demonstrated by the potential temperature θ'_w in convective or frontal regions. It is assumed that the liquid water droplets or ice crystals are withdrawn from cloud in the form of precipitations species as far as they are created by condensation processes. These are irreversible kind of processes, and parts of the entropy are withdrawn by precipitation.

The consequence is that the conservative properties assumed for θ_e or θ_{es} do not correspond to the Second Law of thermodynamics applied to a specific parcel of moist air. It corresponds to the change in entropy expressed per unit mass of dry air of a moist parcel, and so making it useless for applications to a barycentric vision and to the computation of material derivatives of moist air. Another drawback linked to the choices of $PV(\theta_e)$ or $PV(\theta_{es})$ is that the associated solenoidal terms does not cancel out, and that these equivalent potential vorticities are not invertible.

Another “saturation equivalent” potential temperature θ_e^* is defined in S04. It is built in order to cancel the solenoidal term, and like θ_v it is invertible under balanced conditions, but it does not have the correct limit in the dry-air case – i.e. $PV(\theta)$ – making it “useless for general applications”, according to the author.

Taking into consideration the advantages and drawbacks described in S01 and S04, the method followed in the next section will consist of modifying the existing moist air approaches by seeking a new specific (i.e. per unit of moist air) ψ function to be put into (1) and (2) and which could satisfy moist conservative properties (i.e. for which changes in material derivative are caused by pure diabatic processes).

3 The moist entropy.

The aim of the present article is to express the formulation (1) in terms of the specific moist air entropy, namely with $\psi = s$. The moist air entropy is expressed in M11 in terms of a potential temperature θ_s , according to the relationships

$$s = s_{ref} + c_{pd} \ln(\theta_s), \quad (16)$$

$$(\theta_s)_1 = \theta \exp\left(-\frac{L_v q_l + L_s q_i}{c_{pd} T}\right) \exp(\Lambda_r q_t), \quad (17)$$

$$\theta_s = (\theta_s)_1 \left(\frac{T}{T_r}\right)^{\lambda q_t} \left(\frac{p}{p_r}\right)^{-\kappa \delta q_t} \left(\frac{r_r}{r_v}\right)^{\gamma q_t} \frac{(1 + \eta r_v)^{\kappa(1 + \delta q_t)}}{(1 + \eta r_r)^{\kappa \delta q_t}}. \quad (18)$$

The formulation (16) provides a definition (18) for θ_s which is different from the definition obtained for θ_e from (11).

The dimensionless Λ_r -term is defined in M11 by

$$\Lambda_r = \frac{(s_v)_r - (s_d)_r}{c_{pd}} \approx 5.87. \quad (19)$$

This term Λ_r depends on the difference between the reference values $(s_v)_r$ and $(s_d)_r$ for dry air and water vapour, respectively. Therefore Λ_r depends on the reference values T_r , p_r and e_r .

However, it is explained in M11 that the other terms in the full formulation (18) rearrange so that θ_s is really independent on the reference values. It is thus equivalent to the specific moist-air entropy state function and it may be computed locally.

A justification for studying θ_s as a relevant meteorological variable is given in M11. Investigations of the thermodynamical internal structure of several marine stratocumulus demonstrate that, even if the clear-air and in-cloud vertical profiles of the basic variables are not homogeneous, the vertical gradients of thermal and water content properties combine so that the moist entropy and θ_s are almost constant within the PBL and the top-PBL entrainment region.

It is shown in M11 and in Marquet and Geleyn (2013) that θ_s can be accurately represented by the approximation $(\theta_s)_1$ given by (17) and with the typical value of about 5.87 for Λ_r . If ice water content is zero, this approximate formulation only depends on the two well-known moist conservative variables θ_l and q_t (Betts, 1973), with the result

$$(\theta_s)_1 = \theta_l \exp(\Lambda_r q_t) . \quad (20)$$

In order to avoid misinterpretations, the exact formula (18) for θ_s will be used in the next sections to define and compute the new moist potential vorticity components $PV(s)$, denoted by PV_s . The small impact of the approximation of θ_s by $(\theta_s)_1$ will be demonstrated by comparing the corresponding exact and approximate versions of PV_s in Section 8 and in Appendix B.

4 The new moist PV components.

The aim of this section is to compare the formulation $PV(\theta_v)$ studied in S01 with a new formulation $PV(s)$ computed with the moist entropy given by (16)-(19).

Since c_{pd} and s_{ref} are constant terms, the quantity $PV(s)$ is equal to $c_{pd} PV[\ln(\theta_s)]$. The moist entropy represented by $c_{pd} \ln(\theta_s)$ is thus a fundamental specific quantity associated with the Second Law.

Let us consider the identity

$$c_{pd} \ln(\theta_s) = c_{pd} \ln(\theta_v) + c_{pd} \ln(\theta_s/\theta_v) . \quad (21)$$

The choices of $\psi = c_{pd} \ln(\theta_v)$ and $\psi = c_{pd} \ln(\theta_s)$ correspond to the exact differential properties

$$c_{pd} d[\ln(\theta_v)] = c_{pd} \frac{d\theta_v}{\theta_v} , \quad (22)$$

$$c_{pd} d[\ln(\theta_s)] = c_{pd} \frac{d\theta_s}{\theta_s} . \quad (23)$$

In contrast with the differential $d\theta_v$ and the formulation $PV(\theta_v)$ studied in S01, the division by the potential temperature θ_v and the multiplication by c_{pd} in (22) imply a change of unit and a change in magnitude.

More precisely, if $PV(\theta)$ and $PV(\theta_v)$ are expressed with the standard unit of $10^{-6} \text{ m}^2 \text{ K s}^{-1} \text{ kg}^{-1}$ (i.e. the PVU), a possible unit for $PV(s)$ may be $10^{-6} \text{ m}^4 \text{ K}^{-1} \text{ s}^{-3} \text{ kg}^{-1}$. This generates a magnifying factor equal to $c_{pd}/\theta_v \approx 3.5$ to 3 in the troposphere and the lower stratosphere, respectively. This factor decreases toward the values 2.5 and 2 in the upper stratosphere.

Let us define the dry-air entropy, virtual and moist entropy potential vorticities by

$$PV_\theta = \frac{c_{pd}}{3} PV[\ln(\theta)] = \frac{c_{pd}}{3\theta} PV(\theta) , \quad (24)$$

$$PV_v = \frac{c_{pd}}{3} PV[\ln(\theta_v)] = \frac{c_{pd}}{3\theta_v} PV(\theta_v) , \quad (25)$$

$$PV_s = \frac{c_{pd}}{3} PV[\ln(\theta_s)] = \frac{c_{pd}}{3\theta_s} PV(\theta_s) . \quad (26)$$

Division by the factor 3 in the new definitions (24)-(26) is convenient in practice, in order to recover standard values close to 1.5 for PV_θ at the tropopause. This corresponds to a modified moist entropy potential vorticity unit (PVUS) equal to $3 \cdot 10^{-6} \text{ m}^4 \text{ K}^{-1} \text{ s}^{-3} \text{ kg}^{-1}$.

The component PV_s depends, from (26), on the gradient of $\ln(\theta_s) = (s - s_{ref})/c_{pd}$, and thus on the gradient of the specific moist entropy, since s_{ref} and c_{pd} are two constants. Therefore, PV_s observes the same conservative behaviour as the specific moist entropy.

According to S04 it is important to confirm that the dry-air limit of θ_s , which corresponds to $q_v = q_l = q_i = 0$, is equal to θ . This expected result is true, leading to $PV_s = PV_v = PV_\theta$ for a dry-air parcel, a quantity which is proportional to the expected Ertel's formulation $PV(\theta)$, but expressed in terms of the dry entropy and represented by (24). The differences with the Ertel's formulation are the coefficient $c_{pd}/(3\theta)$ and the corresponding change of unit (PVU replaced by PVUS).

The formulation (25) for PV_v can be separated into the sum of two components. The method is to take the logarithm of θ_v given by (10). The result is the sum

$$PV_v = PV_\theta + \frac{c_{pd}}{3} \frac{PV(\delta q_v - q_l - q_i)}{(1 + \delta q_v - q_l - q_i)}. \quad (27)$$

The first component PV_θ is given by (24) and depends on the Ertel's potential vorticity formulation $PV(\theta)$. The second component in (27) depends on $PV[\delta q_v - q_l - q_i]$, a quantity which depends only on the gradient of water contents.

It is possible to compute numerical values of PV_s given by (26) and with the full formulation (18) for θ_s , as demonstrated in the numerical experimentations shown in the next sections. It is more difficult to understand and interpret accurately all the physical properties of the components PV_s , because the expression of θ_s is really complicated, due to all terms in (18) which multiply $(\theta_s)_1$. The component PV_s may be approximated, if needed, by assuming that the moist entropy potential temperature can be approximated by $(\theta_s)_1$ given by (17), as shown in Appendix B.

5 Numerical experimentations.

The French ARPEGE-IFS operational NWP model is used with the stretched and tilted pole configuration and with a zoom coefficient of 2.4 over France. The equivalent truncation is close to T2000 with a maximum resolution of about 10 km over France, Spain and the UK. The resolution is better than 20 km over the whole northern mid-latitudes Atlantic domain. The truncation is close to T333 with a resolution of 60 km over Australia. The model is run with 70 hybrid vertical levels and with a reduced Gauss grid of 800 latitudes.

The mean sea level pressure and the 850 hPa θ'_w fields are depicted in Figure 1(a) for the 21st of September, 2011 (3 hour forecast from 0 UTC). The frontal region extends from the southwest to the northeast of the domain, where it is located over the Channel and the North Sea. The frontal region is roughly delimited by the shaded values of θ'_w higher than 12°C . The northern frontal limit is outlined at 850 hPa as a dashed line, whereas the surface front is associated with the mean sea level pressure trough located in the middle of the 850 hPa frontal region.

The dotted straight line extending from the west of Ireland to the north of Spain represents the cross-section which will be studied in the next sections. It crosses the frontal region at 1020 hPa to the west of France and south of Ireland.

The 850 hPa θ_s field is depicted in Figure 1(b). It is similar to the θ'_w field, provided that the frontal region is defined by values of θ_s higher than 33°C (versus above 12°C for θ'_w) and if contours of θ_s are plotted every 3°C (versus every 2°C for θ'_w).

The upper-levels dynamical fields are shown in Figure 2. The patterns of the geopotential on the $PV(\theta) = 1.5$ PVU surface and the 250 hPa wind speed exhibit elongated features of low

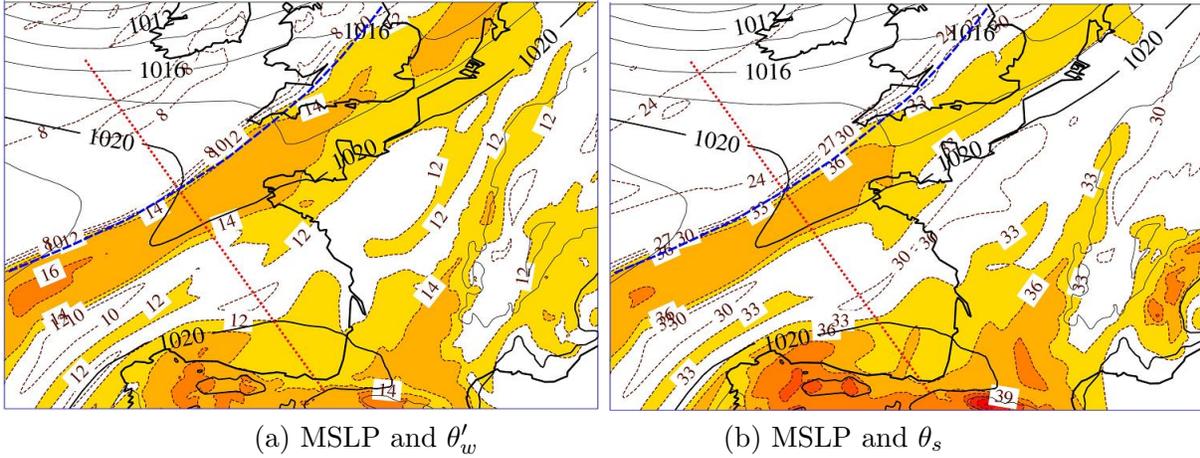


Figure 1: Operational outputs from the ARPEGE-IFS model for 3 hours forecasts from 0000 UTC on 21 September 2011. The horizontal resolution of the post-processed grid is 0.1° (≈ 10 km). Mean sea level pressure (contours every 2 hPa, bold contour for 1020 hPa), and potential temperatures (a) θ'_w at 850 hPa (contour every 2° C, shaded above 12° C), and (b) θ_s at 850 hPa (contour every 3° C, shaded above 33° C). The dotted straight line represents a vertical cross-section extending from the west of Ireland (49° N - 10° W) to northeast of Spain (46° N - 6° W). The dashed line represents the 850 hPa northern frontal limit.

values for the 1.5 PVU geopotential and a significant jet area, both aligned near and to the north of the 850 hPa front. These features indicate that the cross-section is located across the upper air anomalies and to the southwest (rear) of the Jet.

6 Cross-sections of potential temperature.

Cross-sections are plotted in Figures 3(a)-(d) for the potential temperatures θ_v , θ_s , θ'_w and θ_e , respectively. Numerical values of θ_e are computed according to Bolton (1980). The location of the vertical cross-section is depicted in Figures 1 and 2.

The patterns of the frontal region are described differently by each potential temperature. There is almost no signal in (a) with the virtual potential temperature θ_v . This confirms that the difference between θ and θ_v and the impact of moist air on θ_v must be small.

The cross-sections of θ'_w and θ_e exhibit almost the same general pattern in (c) and (d), except that the contours and shaded regions correspond to different values. The frontal limits may be associated with the bold lines $\theta'_w = 14^\circ\text{C} \approx 287$ K or $\theta_e = 42^\circ\text{C} \approx 315$ K, with 850 hPa fronts located in the middle of the cross-section, on each sides of the longitude 8 W.

Almost the same frontal region can be seen in (b) for θ_s and below the level 800 hPa. The bold lines $\theta_s = 33^\circ\text{C} \approx 306$ K delimit almost the same fronts as the bold lines of the pseudo-adiabatic potential temperatures (θ'_w and θ_e), although the fronts are less vertical with θ_s than for the pseudo-adiabatic potential temperatures.

The vertical gradients of θ_s are smaller than the one observed for θ'_w and θ_e outside the frontal region and in the lower part of the planetary boundary layer (PBL; below 850 hPa). Moreover the marked minimum observed close to the level 850 hPa for both θ'_w and θ_e almost disappears for θ_s . This corresponds to the well-mixed regime already observed for the moist-air entropy in the PBL and at the top of the PBL of marine stratocumulus (M11), but verified here for the cold sectors located north and south to the frontal region, where moist turbulence and shallow convection are both active.

The differences are more important above 700 hPa or within the frontal region. The pseudo-

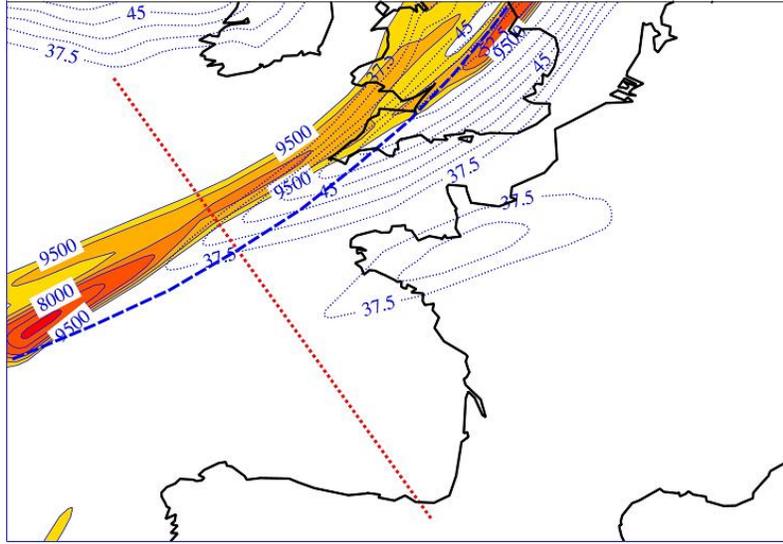


Figure 2: Area as Figure 1, but showing the 250 hPa wind speed (dotted contours every 2.5 m s^{-1} above 37.5 m s^{-1}), and the height of the 1.5 PVU level, computed with the usual Ertel's version $PV(\theta)$ (shaded areas from 5000 to 8000 every 1000 m, then every 500 m up to 9500m).

adiabatic potential temperatures θ'_w and θ_e are almost conserved up to 600 hPa within the frontal region, whereas a vertical gradient of θ_s exist over the the whole frontal region, from 900 hPa to 400 hPa. These differences can be explained by the different impacts of physical processes. On the one hand, specific moist entropy increases with height, because vertical gradients of θ_s demonstrate the impact of irreversible or pseudo-adiabatic processes on moist entropy. On the other hand, θ'_w and θ_e are conserved by deep-convection saturated and precipitating processes, because they have been defined for this purpose as conserved quantities, but expressed per unit mass of dry air.

It is worth remarking that contours of θ_s in (b) are different from those of θ_v in (a) up to the 400 hPa level, and especially in the moist warm sector. This can be explained by the term $\exp(\Lambda_r q_t)$ which multiplies θ_l – i.e. almost θ – and impacts largely on θ_s in spite of the decreasing values of q_t , due to the large value of $\Lambda_r \approx 5.87$ which is about 10 times larger than $\delta \approx 0.608$, i.e. the term acting on q_v in the moist formulation (10) for θ_v . The same impacts are observed in the warm sector of θ'_w and θ_e between 600 and 400 hPa.

7 Isobaric charts of potential vorticities.

The horizontal structures of the moist potential vorticities PV_v , PV_e and PV_s at 850 hPa are shown in Figure 4(a)-(c).

In (a), the PV_v field exhibits smooth structures, with shaded positive regions and values greater than +0.5 PVUS almost everywhere (except in the south of France). The frontal region seems to be associated with an elongated region of positive values above 1 PVUS located at the north of the northern limit (shaded line), with a less organized region located over the north-west of France.

In (b), the pattern of the PV_s field is dominated by the white (unshaded) areas of moderate positive values (between 0 and +0.5 PVUS). An interesting feature is the marked minimum close to the frontal limit, with an elongated feature of negative values less than -2 PVUS in the southwest of Cornwall. This region is the one located below the entrance of the jet and almost below the elongated upper-air anomalies of PV . The cross-section intersects the front within this elongated region of negative values of PV_s . It may corresponds to slantwise convection

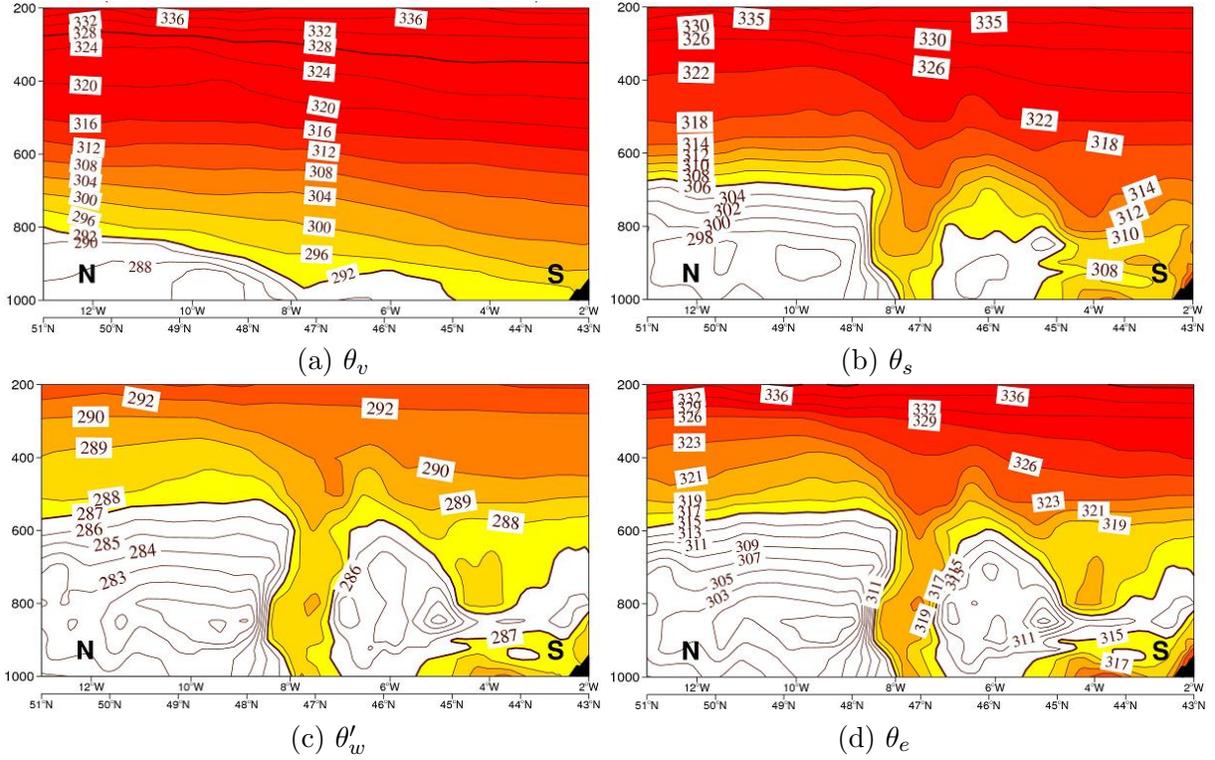


Figure 3: Vertical cross-section computed along the dashed lines depicted in Figures 1 and 2 for (a) θ_v , (b) θ_s , (c) θ'_w and (d) θ_e (Bolton, 1980). The orography of Spain appears at the Southern end. Potential temperatures are in K. Frontal regions are delimited by the shaded regions at $\theta_s > 33^\circ\text{C}$, $\theta'_w > 14^\circ\text{C}$ and $\theta_e > 42^\circ\text{C}$. Post-processed levels are at 1000, 950, 925, 900, 850, then every 100 hPa from 800 to 200 hPa.

instabilities, depending on the sign of the vertical gradient of θ_s . This possibility will be analyzed in more detail in Section 9.

In (c), the use of θ_e leads to large shaded regions of negative values of PV_e (surrounded by dashed lines) almost everywhere. There are only few positive shaded areas of $PV_e > +0.5$ PVUS (surrounded by solid lines). The values of PV_e are thus more negative than those for PV_s . They are lower than -4 PVUS in the same elongated region already observed for PV_s , close to the frontal limit and below the upper-level anomalies.

The interesting feature is that values of PV_s exhibit the same significant negative regions than those of PV_e , but with more moderate negative values, and with almost no negative values elsewhere in the domain. This may be an important property to avoid the instabilities observed in inversion algorithms based on $PV(\theta_e)$, because too negative values make the inversion operator hyperbolic and unstable.

8 Cross-sections of potential vorticities.

Vertical cross-sections as in Figure 3 are shown in Figures 5(a)-(d) for the moist potential vorticity functions PV_v , PV_s , PV_{s1} and PV_e , respectively.

The four moist potential vorticities generate almost the same features above the mid-troposphere, at the tropopause and in the stratosphere, i.e. at and above 500 hPa. For instance, the stratospheric dry-air intrusions into the upper troposphere are almost the same for each potential vorticity (dark shading of values greater than 0.75 and 1 PVUS).

This cannot be explained by small values of q_t observed above 500 hPa, because they are large

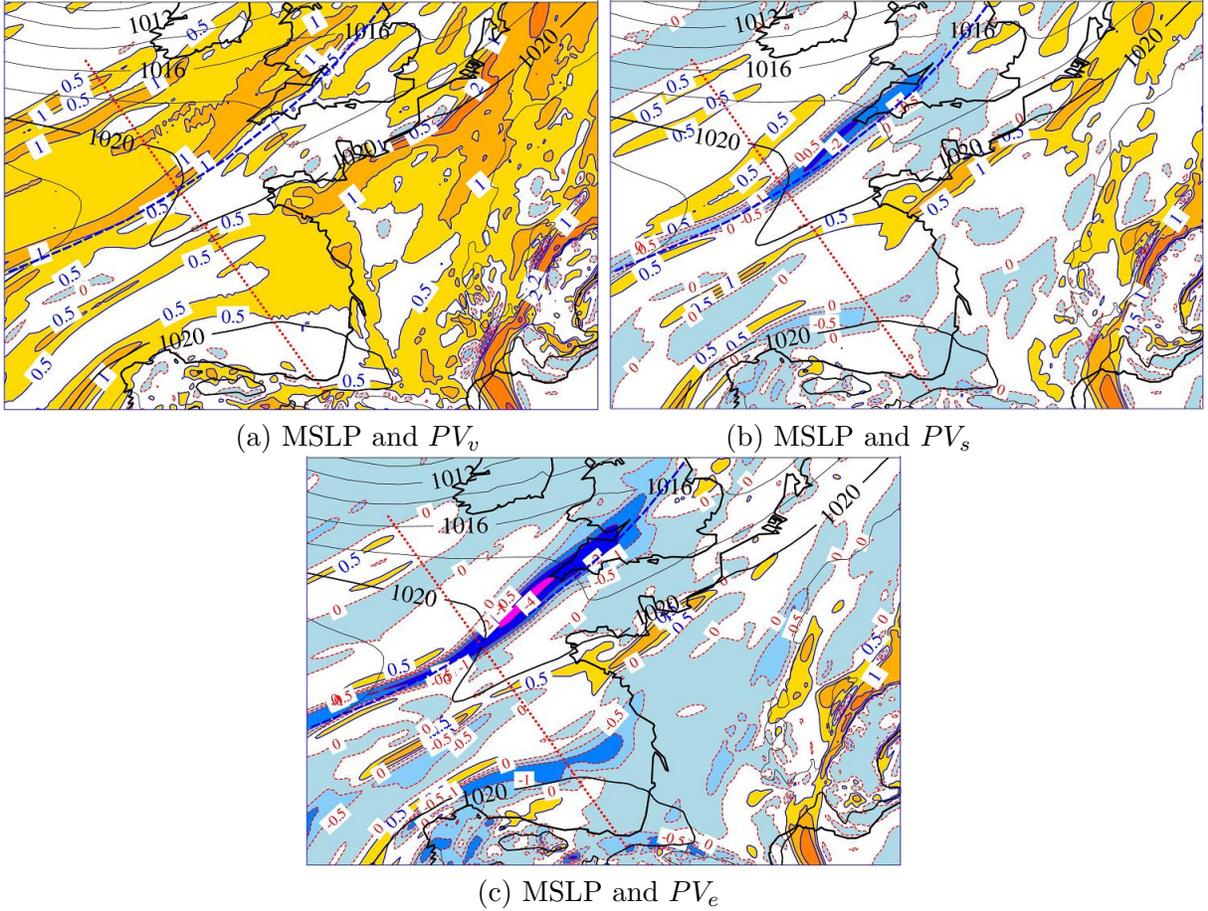


Figure 4: As in Figure 1, but showing the potential vorticity components plotted every 0.5 PVUS at 850 hPa for (a) the virtual component PV_v , (b) the moist entropy component PV_s , and (c) the equivalent component PV_e . Shaded regions represent values of $PV > +0.5$ PVUS (solid contours) or $PV < 0$ PVUS (dashed contours).

enough in the warm sector (located close to 8°W) to make θ_v different from the other components at 400 hPa, as explained in section 6. The explanation is that the differences in potential temperatures mentioned in Section 6 are observed for the horizontal gradients, whereas the vertical gradients are almost the same. And since vertical gradients of potential temperature multiply the large and dominating vertical component of absolute vorticity, the horizontal gradients of potential temperatures generate small terms in potential vorticity components.

Differences can be observed for moist-air potential vorticity components below 500 hPa. The wide shaded regions observed in (a) corresponds to positive values of PV_v greater than 0.5 PVUS. They are not observed for the other components in (b) to (d), where white areas correspond to values between 0 and 0.5 PVUS.

Larger differences are observed in the lower troposphere, below 700 hPa. Whereas values of PV_v are positive everywhere, the frontal limits are associated with moderate negative values of PV_s and with large negative values of PV_e . This confirm the results observed in the 850 hPa charts described in Section 7. These results are valid for other vertical levels, with a vertical extent of negative values of PV_e which is larger than for the moist entropy component PV_s , especially within the warm sector, close to 8°W .

The component PV_{s1} depicted in (c) is the same as PV_s depicted in (b) and given by (26), but with θ_s replaced by $(\theta_s)_1$, giving $PV_{s1} = [c_{pd}/\{3(\theta_s)_1\}] PV[(\theta_s)_1]$. The comparison of the two exact and approximate versions shows very small differences. Examples of these small differences are indicated by small arrows in (c). This is a confirmation that the results obtained in M11,

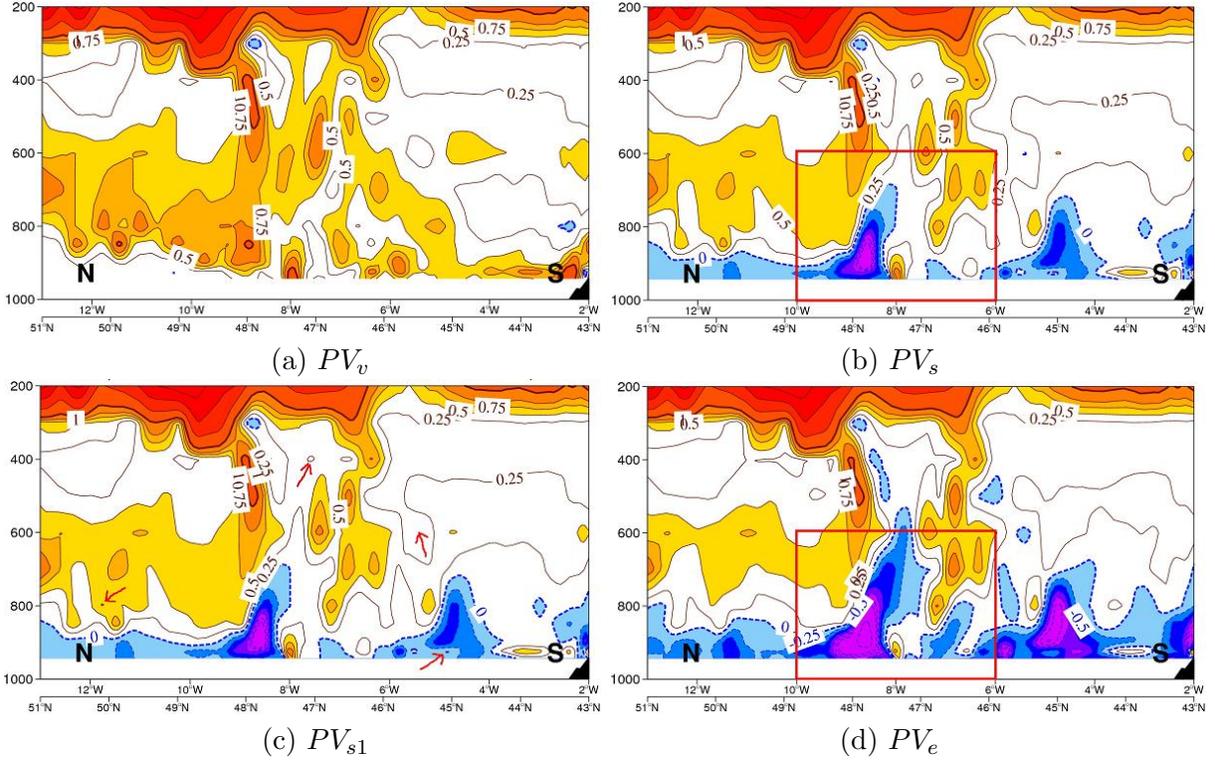


Figure 5: *Cross-sections as in Figure 3, but for the new potential vorticity components (a) the virtual component PV_v , (b) the moist entropy component PV_s , (c) the approximate moist entropy component PV_{s1} , (d) the equivalent component PV_e . Potential vorticities are plotted at 0.25 PVUS intervals between -1.5 and 1 PVUS, with selected uneven values otherwise ($-10, -7.5, -5, -3$ and $1.5, 3, 5, 7.5, 10$ PVUS). Values $> +0.5$ PVUS and < 0 PVUS are shaded, with dashed contours ≤ 0 . The boxes in (b) and (d) represent a sub-region which is used in Figure 7.*

that $(\theta_s)_1$ is indeed a relevant approximation for θ_s , is also valid for the computations of the associated potential vorticities.

It is worth comparing the dry-air versions $PV(\theta)$ and PV_θ with the virtual component PV_v , in order to demonstrate that the previous comparisons of PV_s and PV_e with PV_v can be extended to $PV(\theta)$, the form of PV used in most operational inversion tools. The three fields of $PV(\theta)$, PV_θ and PV_v are plotted in Figure 6. The three fields are almost superimposed for the selected contours (0.5, 1, 1.5, 3, ...) and the lower-level contours of 0.5 PVUS are almost the same. This is another way to show that the impact of q_t on θ_s , and thus on PV_s , is much smaller than the impact of q_t on θ_v , and thus on PV_v , as explained at the end of Section 6.

9 Slantwise convection.

According to the criteria described in BH79, conditional symmetric instability and slantwise convection may occur in those regions where negative values of PV correspond to positive vertical gradients of potential temperature. In order to better motivate, and to find justification for, the use of PV_s rather than PV_v or PV_e in future inversion tools, we plot on the same figures the potential vorticity components and the vertical gradient of the associated potential temperature. The aim is to find areas where the criteria for slantwise convection might be observed for θ_s , whereas they are not verified with θ or θ_e .

PV_s and the vertical gradient of θ_s are both plotted on Figure 7(a). PV_e and the vertical gradient of θ_e are plotted on Figure 7(b). These cross-sections correspond to the boxes depicted in Figures 5(b,d), between 10 and 6°W and below 600 hPa.

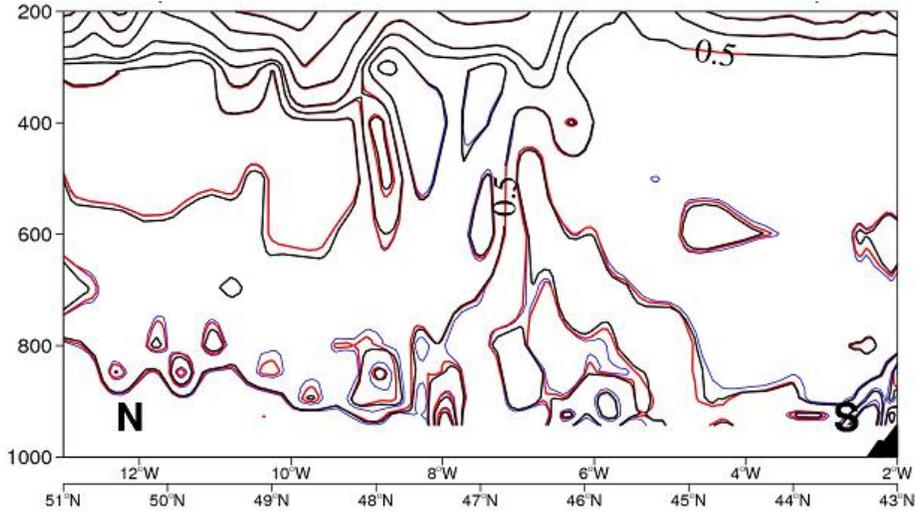


Figure 6: Cross-sections as in Figure 5(a), comparing Ertel's formulation $PV(\theta)$ (plotted every 0.25 PVU), PV_θ and PV_v (plotted every 0.25 PVUS).

In (b), the negative values of PV_e (dashed contours) correspond to negative vertical gradients of θ_e (white regions), indicating that vertical instabilities took place, rather than slantwise convection. Conversely, in (a) negative values of PV_s partly correspond to positive vertical gradients of θ_s (light shaded region). This is true for the north and south frontal limits, at 9 and 7°W. This may indicate that conditional symmetric instability may occur and that slantwise convection may take place in these regions.

An interpretation for these results is that θ_s surfaces are more vertical than θ surfaces in the lower troposphere, but they are less vertical than θ'_w or θ_e surfaces, in a possible proportion of about 2/3 between θ and the pseudo-adiabatic potential temperatures. This proportion of 2/3 is the one observed between $(\theta_l, \theta_s, \theta_e)$ in M11 for the marine stratocumulus.

This property can be used to place the surface of constant θ_s on Figure 2 of BH79. The θ_s surface must be closer to the absolute vorticity vector surface than the θ'_w surface. This could explain why the negative values of PV_s are smaller than the one of PV_e , because this implies that the 3D absolute vorticity vector and the vector of 3D gradient of θ_s are more normal to each other than for the 3D gradient of θ'_w and θ_e .

Another phenomenon may balance the impact due to change of slope of these surfaces. A change in numerical value of the potential temperature may modify the magnitude of the gradient vector, and thus the value of potential vorticity. It could be inferred from Figures 3(b)-(d) that the magnitude of the gradient of θ_s is not larger than those of θ_e , for instance at 48°N and below 900 hPa, within that region of negative values of PV_s and PV_e .

The interpretation of the change of sign for the vertical gradients of θ_s and θ_e (close to 48°N and between 900 and 800 hPa) requires refined analyses and comparisons of the Figures (3)(b) and (d). The θ_e surfaces are oriented so that θ_e decreases with height, whereas θ_s surfaces are almost vertical, so that θ_s is indeed almost neutral, or slightly increases with height.

The main problem to be solved is that the criteria for conditional symmetric instability and the possibility of slantwise convection cannot depend on the choice of θ_s , θ'_w or θ_e to be used in the definitions of the associated vertical gradients and the potential vorticities.

A first remark is that the diabatic sources and sinks appearing in the entropy equation ds/dt are better represented by $d\theta_s/dt$ than by $d\theta'_w/dt$ or $d\theta_e/dt$. The explanation is given in section 2: θ'_w or θ_e are expressed per unit mass of dry air, whereas material derivatives and barycentric formulations require a specific definition for the moist entropy of moist air. This requirement is displayed only by θ_s introduced in M11 and covered in Section 3.

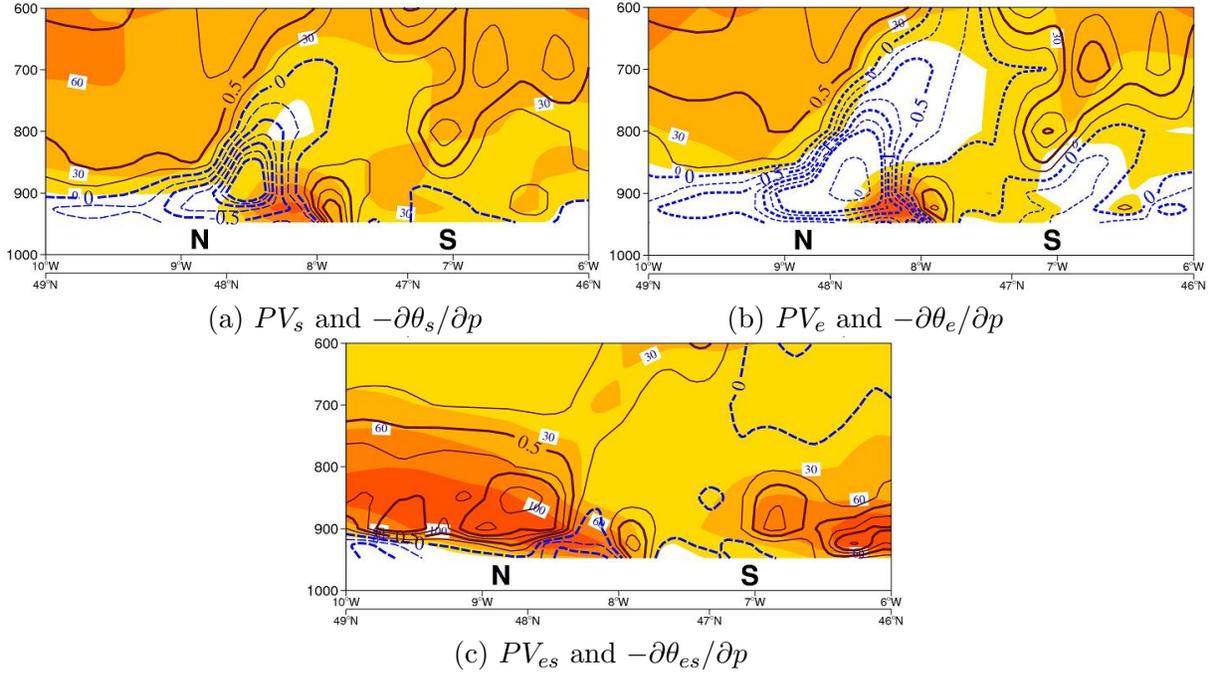


Figure 7: Cross-sections over the sub-area depicted by boxes in Figures 5(b) and (c) showing PV components and vertical gradients ($-\partial\theta/\partial z$) for: (a) PV_s and (θ_s) , (b) PV_e and (θ_e) (Bolton, 1980), and (c) PV_{es} and θ_{es} given by (9). Potential vorticities are plotted every 0.25 PVUS intervals (solid contours if > 0 , dashed if ≤ 0). Vertical gradients are depicted as light shaded areas for positive values, and darker shading above 30, 60 and 100 units of $K(1000 \text{ hPa})^{-1}$.

The patterns of $PV_{es} = [c_{pd}/(3\theta_{es})] PV(\theta_{es})$ in Figure 7(c), where θ_{es} is defined by (9), are very different from those of PV_e in (b). Values of potential vorticities and vertical gradients are thoroughly modified in the lower troposphere. The consequence is that PV_{es} defined in terms of θ_{es} cannot be used from a forecaster’s viewpoint.

It is thus tempting and logical to modify the method initiated in BH79 and to define a reduced static stability expressed by $N_s^2 = (g/\theta_r)(\partial\theta_s/\partial z)$ and a corresponding entropic potential vorticity by $PV(\theta_s)$ or PV_s , with θ_s replacing θ'_w , θ_e or θ_{es} . The motivations are the same as in previous articles: to get a moist-air generalization of Ertel’s potential vorticity by specifying the specific moist-air entropy, with the new result that θ_s should be used if all the properties of moist air entropy are to be taken into account. It may be worthwhile to notice that N_s^2 somehow corresponds to the entropy part of the squared Brunt-Väisälä frequency computed in Marquet and Geleyn (2013), provided that a positive factor in front of N_s^2 is approximated by 1, in the same way as the positive term Γ_m/Γ_d is often discarded in the formulations which use θ'_w or θ_e .

10 Charts of low-levels potential vorticities.

The moist-air potential vorticity components PV_v , PV_s and PV_e are compared in Figures 8(a)-(f) for a large Atlantic domain, extending from the west of Europe to the Canada. Values of potential vorticities are averaged for three low levels below 900 hPa, in order to be less sensitive to numerical problems and to get more significant results. The shaded regions represent the warm sectors and occluded fronts. They are delimited by the threshold $\theta'_w > 12^\circ\text{C}$ and with darker shaded areas for higher values of θ'_w .

Solid or dashed lines of equal values of PV_v , PV_s and PV_e form coherent signals which are associated with most of the midlatitudes fronts and low-latitudes thermal limits. These signals do not exhibit random or noisy patterns. They are advected with the eastward general circulation

and they remain close to the same parts of fronts and thermal limits.

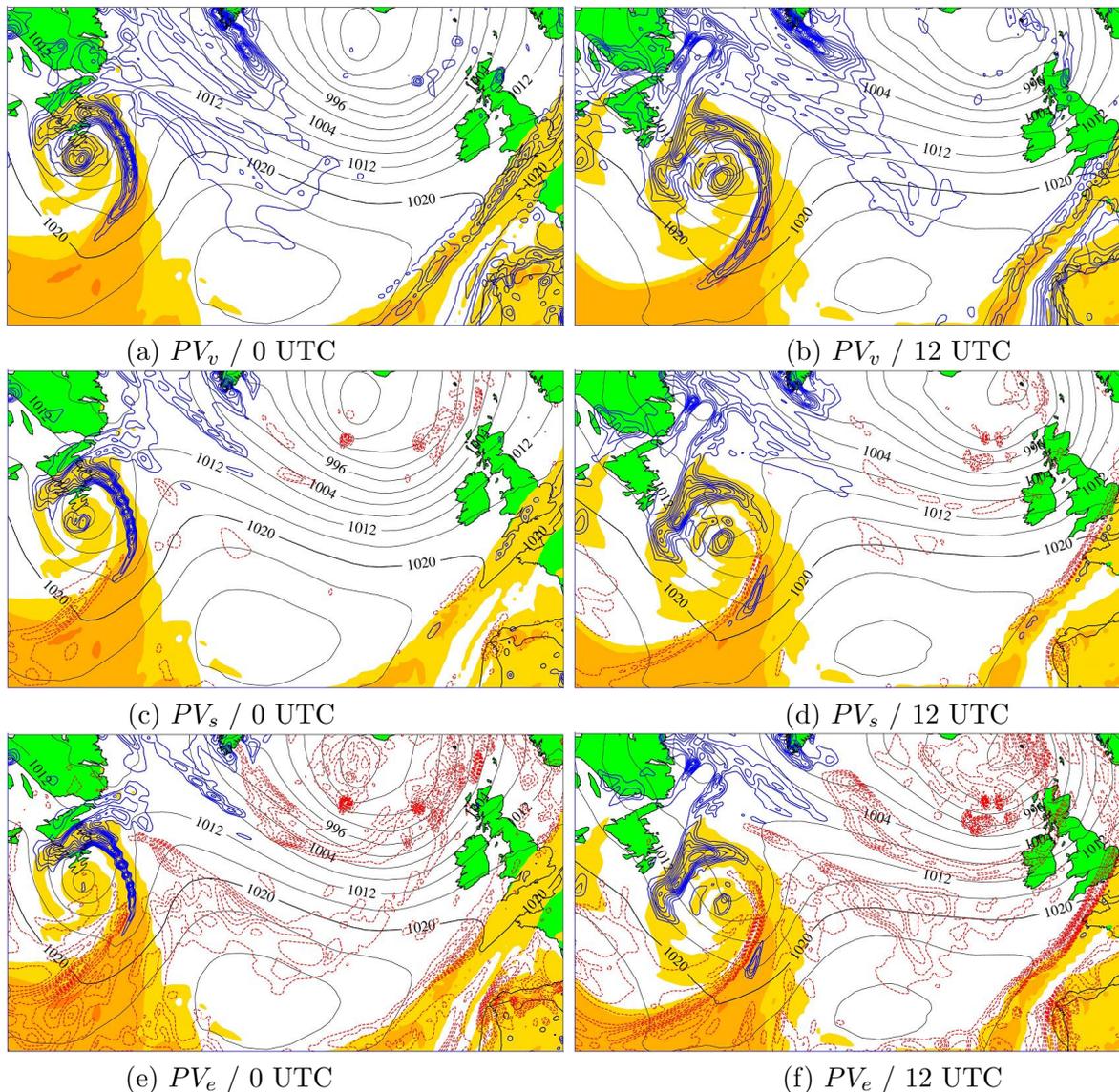


Figure 8: Operational output from ARPEGE-IFS model showing analyses and forecasts from 0000 UTC on 21 September 2011. The horizontal resolution of the post-processed grid is 0.5° everywhere, although the resolution of the variable mesh ARPEGE model is about 10 km over France, Spain and England and about 20 km over the eastern part of the domain. MSLP is plotted every 4 hPa, with a bolder contour for 1020 hPa. The potential vorticities are average for the levels 900, 925 and 950 hPa, for a) PV_v at 0000 UTC, b) PV_v at 1200 UTC, c) PV_s at 0000 UTC, d) PV_s at 1200 UTC, e) PV_e at 0000 UTC, and f) PV_e at 1200 UTC. Values of $|PV|$ are plotted above the threshold 0.5 PVUS and then every 0.25 PVUS intervals. Positive solid contours are in blue, and negative dashed contours are in red. Values of θ'_w at 850 hPa are represented by (yellow and orange) shaded regions above the threshold 12, 14 and 16°C.

Charts of PV_v are dominated in (a) and (b) by positive values close to the fronts (solid lines), with a wide region of weak positive values located over the central North Atlantic. Charts of PV_e are dominated in (e) and (f) by negative values (dashed lines), for instance in the central Atlantic, except over warm or occluded fronts where elongated positive structures can be observed.

Charts of PV_s are more balanced in (c) and (d), with the North Atlantic almost free of potential vorticity signal. Localized and elongated dipole structures are observed close to the cold fronts, with negative values of PV_s on the west side. The same elongated regions of positive values as the ones observed for PV_e are localized above the warm or occluded fronts. This suggests an interpretation of these PV_s features in terms of the T-bone structure described in Shapiro and

Keyser (1990), with fracturing of the frontal zone near low center. It would be interesting to analyze further these signals of moderate negative values of PV_s , and to determine if they could be associated with intensifying fronts. For instance, according to forecasters' analyses reported on PRESYG charts (Santurette and Joly, 2002), the elongated structure located on the central North Atlantic toward Ireland can be associated with pseudo-warm fronts.

The conclusion of this section is that the descriptions of the meteorological fields in terms of PV_v , PV_s or PV_e are not equivalent. They correspond to different dynamic, thermal and moist aspects of the atmosphere. It seems that it is easier to analyze the frontal structures of PV_s than those described by PV_v or PV_e . This result may signify that it is indeed important to base the computation of moist-air potential vorticity on the Second Law formulation $c_{pd} \ln(\theta_s)$.

11 Hints for inversion methods for PV_s .

It is well-known that an inversion method requires:

- i) an invertible equation, preferably elliptic or not too far hyperbolic;
- ii) a relevant set of N equations corresponding to N state variables and;
- iii) suitable boundary conditions.

The main purpose of the present article is to analyze the diagnostic properties displayed by θ_s and the associated potential vorticity PV_s . Even though a realistic method may or may not exist to invert PV_s , this section and Appendices C and D analyze the possibility of using PV_s in some way as a starting point for future inversion tools.

A first approach may correspond to the results derived in S01 and S04, where it is demonstrated that PV_v demonstrates a moist-air invertibility principle (although it is not possible to determine all the moist air variables after the inversion process). It is possible to rely on this property and to control the invertible quantity PV_v expressed as a sum of the specific moist-air entropy version PV_s plus a new component PV_q :

$$PV_s = PV_v + PV_q, \quad (28)$$

$$PV_q = \frac{c_{pd}}{3} PV[\ln(\theta_s/\theta_v)] . \quad (29)$$

This expression for PV_q results directly from (25) and (26). It depends on the gradients of $\ln(\theta_s/\theta_v)$. It is explained in Appendix B that the quotient θ_s/θ_v mainly depends on the gradients of the water contents q_t , q_l and q_i , giving the explanation for the notation PV_q . The dry-air limit of PV_q is equal to 0, since $PV_s = PV_v$ in that case. The consequence is that PV_q observes an adiabatic (closed) conservative property associated with the joint conservation of the dry-air and water contents q_d and q_t , as far as the impact of q_l or q_i is small. A similar component $PV(q_v)$ has been defined and studied in Gao and Zhou (2008).

The reason why it may be easier to manage the sum $PV_s + PV_q$ than PV_v alone is that:

- i) upper-air patterns of PV_s correspond to the well-known analysis of anomalies of PV_θ or PV_v located above 600 hPa, as shown in Figures 5(a)-(b);
- ii) lower-tropospheric signals can be easier analyzed with PV_q below 600 hPa.

The last property can be verified by analyzing the chart of PV_q at 850 hPa shown in Figures 9(a) and the cross-section of PV_q depicted in Figures 9(b). Values of PV_q are negative almost everywhere in (a) and (b). The limit -0.25 PVU extends up to 400 hPa within the northern limit of the tilted frontal region only, with other significant values of PV_q observed within the lower troposphere only (below 700 hPa). A tilted region of positive values are observed close to the southern limit of the front. It extends up to 300 hPa close to 7°W and between 46 and 47°N .

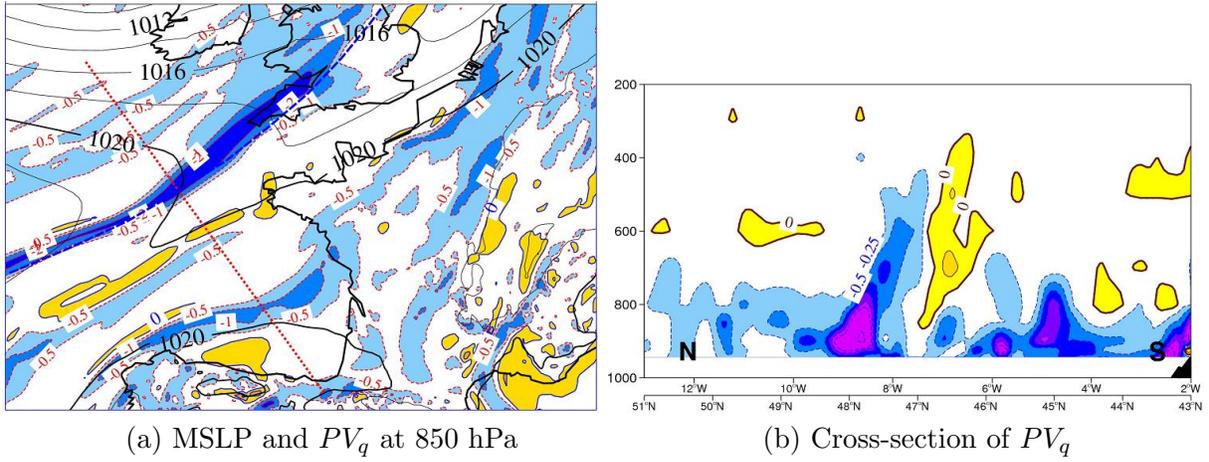


Figure 9: Chart and cross-section as in Figures 4 and 5, but for the potential vorticity PV_q given by (29). Values of PV_q are shaded for positive values (with solid contours) and for negative values (dashed contours) ≤ -0.5 PVUS in (a), and ≤ -0.25 PVUS in (b).

A second approach may follow from inversion processes directly applied to the specific moist-air entropy potential vorticity PV_s . The steps of analysis and modifications of the PV_s field could rely on the separation observed in Figure 4(b) and 5(b) between upper-troposphere positive values versus lower-troposphere negative values, mostly associated with the frontal regions.

The advantage of PV_s with respect of PV_e is that θ_s observes the Second Law conservative property applied to the specific moist-air entropy, whereas θ_e does not, since it is not based on a specific quantity. The drawback associated with the use of PV_s is that the solenoidal term defined by the term in the right-hand side of the first line of (2) does not cancel out with $\psi = \theta_s$, whereas it does with $\psi = \theta_v$.

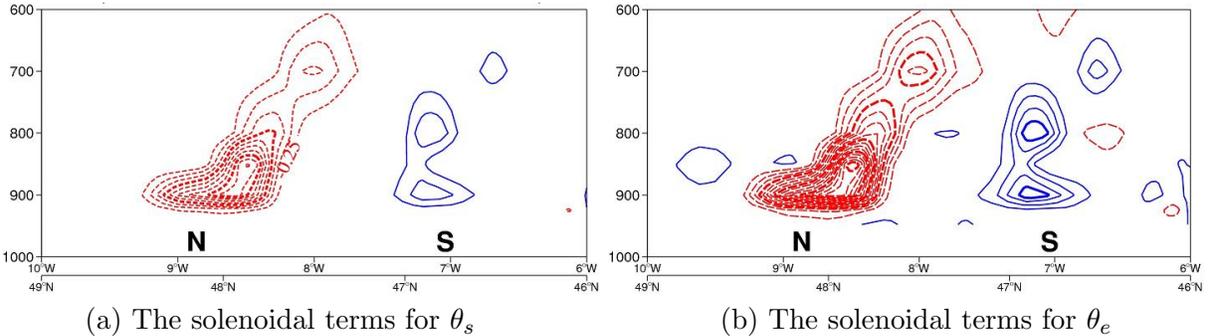


Figure 10: Cross-sections as in Figures 7, but for the solenoidal terms (units $10^{-10} \text{ m s}^{-4} \text{ K}^{-1}$) for (a) θ_s , and (b) θ_e . Contours are shown at 0.25 unit intervals, with solid (blue) contours ≥ 0.25 and dashed (red) contours ≤ -0.25 .

However, the same problem exist in inversion methods applied to PV_e , with $\psi = \theta_e$ generating a non-cancelling solenoidal term. Numerical values of the two solenoidal terms generated by $\psi = \theta_s$ or θ_e are compared in Figures 10(a,b).

The promising result is that the solenoidal term obtained with θ_s is about half that obtained with θ_e . It has been confirmed (not shown) that the solenoidal terms obtained with θ and θ_v are, as expected, very small in comparison with that obtained with θ_s (10 times lower with θ and 1000 times lower with θ_v).

The problem generated by the non-vanishing solenoidal term is thus less important with PV_s than with PV_e . The problem of the non-elliptic character for the inversion operator may also be less important with the observed moderate negative values of PV_s , in comparison with the larger

negative values for PV_e .

12 Conclusions.

The purpose of this article was to define a moist potential vorticity PV_s written in terms of the specific moist entropy and the potential temperature θ_s described in M11. An associated new PV unit has been derived, in order to recover the same numerical values of about 1.5 PVUS at the tropopause, where dynamical anomalies are classically analyzed with Ertel's component PV_θ .

Outputs from a NWP model are used to illustrate and analyze the spatial and temporal patterns of the new moist-air potential vorticity PV_s . The other formulations PV_v and PV_e obtained with the well-known virtual and equivalent potential temperatures θ_v and θ_e are compared with PV_s .

Analyses of isobaric charts and vertical cross-sections show that:

- i) the upper level positive anomalies of PV_s are similar to the well-known Ertel's PV_θ structures;
- ii) the low-level features are associated with frontal regions and with moderate negative values (about half the values of PV_e);
- iii) the low level properties displayed by PV_s close to the fronts might be associated with the criteria which control conditional symmetric instability and slantwise convection;
- iv) the low level solenoidal term generated by PV_s is half the one generated by PV_e .

The main justification for the use of PV_s in place of PV_e is that the conservation principle associated with the Second Law must be expressed with material derivatives of a specific moist-air quantity. It is explained that neither θ'_w nor θ_e fulfils this requirement, because they are associated with pseudo-adiabatic processes expressed by unit mass of dry air, not with specific values. One could say that " θ'_w and θ_e are pseudo-adiabatically conserved quantities which are not conservative, whereas θ_s is the conservative variable associated with the specific moist air entropy which is conserved for closed, adiabatic moist-air processes".

It is possible to define a water potential vorticity PV_q computed as the difference between PV_s and the virtual value PV_v . It is shown that spatial structures of low-level negative values of PV_s are highlighted by PV_q , with larger negative values which may be used to analyze, modify and control those low-level signals which are more difficult to see with PV_s , and are even absent in PV_v .

The main interest for introducing the water component PV_q would be that it may allow a partition of the invertible component PV_v into a weighting sum of the Ertel's PV and PV_q , each of them controlling different, separated parts of the atmosphere. This partition may be a relevant one, since the virtual potential vorticity PV_v seems to be the only moist air PV which demonstrates an invertibility principle.

It could be interesting to test alternative inversion methods based on PV_s alone, with the positive upper-level and negative lower-level structures which could be analyzed, modified and controlled with the same horizontal charts and vertical cross-sections of PV_s as shown in the paper.

More sophisticated numerical modelling and observational studies of PV_s are required to assess the possibility of a realistic inversion tool based on PV_s alone, or on the pair of potential vorticities PV_θ and PV_q .

As a final perspective, it may be possible to improve the variational moist inversion method described by Arbogast *et al.* (2008) and based on the ideas of Vallis (1996), by testing for instance a moist total available enthalpy norm to solve the corresponding variational problem, with the moist entropy used in the present paper entering the moist norm. It will be necessary to derive an associated moist quasi-geostrophic set of equations, with prognostic equations for water species

which might correspond to the moist entropy and water components PV_s and PV_q defined here.

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Appendix A. List of symbols and acronyms.

α	= $1/\rho$ the specific volume
c_{pd}	specific heat for dry air (1004.7 J K ⁻¹ kg ⁻¹)
c_{pv}	spec. heat for water vapour (1846.1 J K ⁻¹ kg ⁻¹)
c_l	spec. heat for liquid water (4218 J K ⁻¹ kg ⁻¹)
c_i	spec. heat for ice water (2106 J K ⁻¹ kg ⁻¹)
c_p	specific heat at constant pressure for moist air, = $q_d c_{pd} + q_v c_{pv} + q_l c_l + q_i c_i = q_d (c_{pd} + r_v c_{pv} + r_l c_l + r_i c_i)$
C_1, C_2	two terms appearing in a moist entropy equation
c_p^*	a specific heat depending on r_t
δ	= $R_v/R_d - 1 \approx 0.608$
η	= $1 + \delta = R_v/R_d \approx 1.608$
κ	= $R_d/c_{pd} \approx 0.2857$
γ	= $\eta \kappa = R_v/c_{pd} \approx 0.46$
λ	= $c_{pv}/c_{pd} - 1 \approx 0.8375$
e_r	the water vapour reference partial pressure, with $e_r = e_{ws}(T_0) \approx 6.11$ hPa
f	the Coriolis parameter
Λ_r	= $[(s_v)_r - (s_d)_r]/c_{pd} \approx 5.87$
$L_v(T)$	= $h_v - h_l$: Latent heat of vaporisation
$L_s(T)$	= $h_v - h_i$: Latent heat of sublimation
$L_v(T_0)$	= $2.501 \cdot 10^6$ J kg ⁻¹
$L_s(T_0)$	= $2.835 \cdot 10^6$ J kg ⁻¹
N_s^2	a moist-air squared Brunt-Väisälä frequency
p	= $p_d + e$: local value for the pressure
p_r	= $(p_d)_r + e_r$: reference pressure ($p_r = p_0$)
p_d	local dry-air partial pressure
$(p_d)_r$	reference dry-air partial pressure ($\equiv p_r - e_r$)
p_0	= 1000 hPa: conventional pressure
ψ	dummy scalar value
$PV(\theta)$	Ertel's potential vorticity (PVU)
PV_θ	dry-air entropy potential vorticity (PVUS)
PV_v	virtual potential vorticity (PVUS)
PV_e	equivalent potential vorticity (PVUS)
PV_{es}	saturation equivalent potential vorticity (PVUS)
PV_s	moist-air entropy potential vorticity (PVUS)
PV_q	water potential vorticity (PVUS)
PV_{s1}	approximate version for PV_s (PVUS)
PV_{q1}	approximate version for PV_q (PVUS)
PV_{l1}	liquid-water potential vorticity (PVUS)
q_{sw}	saturated vapour content over liquid water
q_{si}	saturated vapour content over ice water
q_w	wet bulb potential vorticity
q_g	entropic potential vorticity

q_{ge}	equivalent potential vorticity
q_d	$= \rho_d/\rho$: specific content for dry air
q_v	$= \rho_v/\rho$: specific content for water vapour
q_l	$= \rho_l/\rho$: specific content for liquid water
q_i	$= \rho_i/\rho$: specific content for ice water
q_t	$= q_v + q_l + q_i$: total specific content of water
r_v	$= q_v/q_d$: mixing ratio for water vapour
r_{sw}	saturated vapour mixing ratio over liquid water
r_r	reference mixing ratio for water species ($\eta r_r \equiv e_r/(p_d)_r$ and $r_r \approx 3.82 \text{ g kg}^{-1}$)
ρ_d	specific mass for dry air
ρ_v	specific mass for water vapour
ρ_l	specific mass for liquid water
ρ_i	specific mass for ice water
ρ	specific mass for moist air $= \rho_d + \rho_v + \rho_l + \rho_i$
R_v	water vapour gas constant ($461.52 \text{ J K}^{-1} \text{ kg}^{-1}$)
R_d	dry-air gas constant ($287.06 \text{ J K}^{-1} \text{ kg}^{-1}$)
R	$= q_d R_d + q_v R_v$: gas constant for moist air $R = q_d (R_d + r_v R_v)$
s	specific moist entropy
s_{ref}	a reference specific entropy
$(s_d)_r$	reference values for the entropy of dry air at T_r and $(p_d)_r$: $6777 \text{ J K}^{-1} \text{ kg}^{-1}$
$(s_v)_r$	reference values for the entropy of water vapour at T_r and e_r : $12673 \text{ J K}^{-1} \text{ kg}^{-1}$
s_e	a specific moist equivalent entropies
s_r^*	a reference moist entropy depending on r_t
S	a specific moist entropy (Hauf and Höller, 1987)
T	local temperature
T_r	the reference temperature ($T_r \equiv T_0$)
T_0	zero Celsius temperature ($= 273.15 \text{ K}$)
θ	$= T (p_0/p)^\kappa$: the (dry-air) potential temperature
θ_v	the virtual potential temperature
θ_l	the liquid-water potential temperature
θ_e	the equivalent potential temperature
θ_{es}	the saturation equivalent potential temperature
θ_e^*	a saturation equivalent potential temperature (Schubert 2004)
θ_S	a moist entropy potential temperature (Hauf and Höller, 1987)
θ_s	the moist entropy potential temperature (M11)
$(\theta_s)_1$	approximate version of θ_s
ζ_a	the absolute vorticity 3D vector
∇	gradient 3D operator
Ω	angular velocity of the Earth (3D vector)
\mathbf{u}	the velocity (3D vector)
\mathbf{F}	frictional force 3D vector

Appendix B. The approximations PV_{s1} and PV_{q1} .

Since it is possible to approximate θ_s by $(\theta_s)_1$, it is worthwhile to determine to what extent PV_s and PV_q may be modified by this approximation. The hope is to obtain simple analytic expressions for PV_s and PV_q which could be easier to manage and possibly to derive easier physical interpretations.

Let us approximate the moist entropy potential temperature θ_s by $(\theta_s)_1$ given by (17). The

analog of (26) and (29) is the exact separation of PV_{s1} into the sum of

$$PV_{s1} = \frac{c_{pd}}{3} PV[\ln\{(\theta_s)_1\}] , \quad (\text{B.1})$$

$$PV_{q1} = \frac{c_{pd}}{3} PV[\ln\{(\theta_s)_1/\theta_v\}] . \quad (\text{B.2})$$

The component PV_{q1} exactly represent the difference between the approximate entropy component PV_{s1} and the invertible one PV_v .

From the definitions (17) for $(\theta_s)_1$ and (24) for PV_θ , the moist entropy component PV_{s1} can be written as

$$PV_{s1} = PV_\theta + \frac{c_{pd}}{3} PV\left(\Lambda_r q_t - \frac{L_v q_l + L_s q_i}{c_{pd} T}\right) . \quad (\text{B.3})$$

The water content component $PV_{q1} = PV_{s1} - PV_v$ can be computed as the difference (B.3) minus (27), or directly with the quantity $\ln\{(\theta_s)_1/\theta_v\}$ evaluated from (10) and (17) and with the Ertel's potential vorticity PV_θ which cancels out between (27) and (B.3), leading to the result

$$PV_{q1} = -\frac{c_{pd}}{3} \frac{PV(\delta q_v - q_l - q_i)}{(1 + \delta q_v - q_l - q_i)} + \frac{c_{pd}}{3} PV\left(\Lambda_r q_t - \frac{L_v q_l + L_s q_i}{c_{pd} T}\right) . \quad (\text{B.4})$$

This expression mainly depends on the gradients of water contents q_v , q_l and q_i , with small impact due to variations of $L_v(T)/T$ and $L_s(T)/T$ with T in the last PV term of (B.4).

It is possible to express PV_v , PV_{s1} and PV_{q1} , given by (27), (B.3) and (B.4), in terms of the variables θ , q_t , q_l and q_i , with q_v expressed as $q_t - q_l - q_i$. The resulting moist PV components are written as

$$PV_v = PV_\theta + \frac{c_{pd}}{3} \delta \frac{\theta}{\theta_v} PV(q_t) - \frac{c_{pd}}{3} (1 + \delta) \frac{\theta}{\theta_v} [PV(q_l) + PV(q_i)] , \quad (\text{B.5})$$

$$PV_{s1} = PV_\theta + \frac{c_{pd}}{3} \Lambda_r PV(q_t) - PV\left(\frac{L_v q_l}{3T}\right) - PV\left(\frac{L_s q_i}{3T}\right) , \quad (\text{B.6})$$

$$PV_{q1} = \frac{c_{pd}}{3} \left(\Lambda_r - \delta \frac{\theta}{\theta_v}\right) PV(q_t) - PV\left(\frac{L_v q_l}{3T}\right) - PV\left(\frac{L_s q_i}{3T}\right) + \frac{c_{pd}}{3} (1 + \delta) \frac{\theta}{\theta_v} [PV(q_l) + PV(q_i)] . \quad (\text{B.7})$$

The first terms on the right-hand sides of (B.5)-(B.7) depend on $PV(\theta)$ and $PV(q_t)$, whereas the other terms depends on the potential vorticities of condensed water $PV(q_l)$ or $PV(q_i)$.

Appendix C. An inversion method for PV_{s1} and PV_{q1} : the non-saturated moist air.

The aim of this Appendix is to make more explicit the second approach suggested at the end of section 11, for the special case of non-saturated moist air.

The interest of an inversion process to be applied to PV_v relies on the capacity to modify this field PV_v in a relevant way before the inversion step. The method is currently used to manage the upper-troposphere and lower-stratosphere anomalies of PV_θ , which are almost the same as those of PV_v in these dry regions.

The problem is different for the low-level PV_v informations, which is clearly not associated with frontal limits, as shown in Sections 7, 8 and 10. The alternative method is to diagnose more clearly the low-level information with the help of the water component PV_{q1} . Comparisons of Figures 5(b) and 9(b) show that almost the same regions of negative values can be diagnosed with PV_s or PV_q , except that the threshold 0 PVUS for PV_s must be replaced by -0.5 PVUS for PV_q .

Accordingly, the aim is to express PV_v as a weighting sum of PV_θ and PV_{q1} , with PV_θ suitable for upper-level analysis and PV_{q1} for lower-level analysis. The non-saturated moist-air version is considered in this section and the computations valid for the saturated moist air will be conducted in the next section. The non-saturated and dry-air cases are different, with *a priori* a large impact of $0 < q_v < q_{sw}$ on the computations of $(\theta_s)_1$, PV_{s1} and PV_{q1} .

The non-saturated version of PV_v and PV_{q1} are obtained from (B.5) and (B.7) for $q_l = q_i = 0$ and for $q_t = q_v$. The result is

$$PV_v = PV_\theta + \frac{c_{pd}}{3} \delta_v PV(q_v), \quad (\text{C.1})$$

$$PV_{q1} = \frac{c_{pd}}{3} (\Lambda_r - \delta_v) PV(q_v). \quad (\text{C.2})$$

The term δ_v is equal to $\delta (\theta/\theta_v) = \delta / (1 + \delta q_v)$ in non-saturated conditions. The next step is to compute $PV(q_v)$ from (C.2) and to put the result into (C.1). The result is PV_v expressed as the weighting sum

$$PV_v = PV_\theta + \left(\frac{\delta_v}{\Lambda_r - \delta_v} \right) PV_{q1}. \quad (\text{C.3})$$

The property (C.3) explains how it is possible to take into account any modified version of the two components PV_θ and PV_{q1} and how they can be recombined, with the coefficient $\delta_v/(\Lambda_r - \delta_v)$ acting on the water component, to give an updated value for PV_v which may enter an inversion process.

Since $\delta = 0.608$ and because q_v is a small term in the atmosphere, values of δ_v remain close to δ . The impact of q_v on δ_v is of the order of $100 \times q_v$ (in per cent), with for instance $\delta_v = 0.6$ for $q_v = 20 \text{ g kg}^{-1}$. The coefficients acting to mix the components PV_θ and PV_{q1} in (C.3) can thus be evaluated with $\delta_v \approx 0.608$ and $\Lambda_r = 5.87$ to give $\delta_v/(\Lambda_r - \delta_v) \approx 0.116$. Even for a large value of $q_v = 20 \text{ g kg}^{-1}$ the coefficients is almost the same: 0.114. A mean value of 0.115 for $\delta_v/(\Lambda_r - \delta_v)$ leads to the result

$$PV_v \approx PV_\theta + 0.115 PV_{q1}. \quad (\text{C.4})$$

The consequence of (C.4) is that a change of 1 PVUS in PV_{q1} implies a small change of 0.1 PVUS in the virtual component PV_v . This means that the modified values of PV_v would always remain relevant ones, even if PV_q is largely modified.

The term Λ_r is a consequence of the Third Law. It has a large impact on the definition of PV_{q1} given by (C.2) and on the associated coefficient $\delta_v/(\Lambda_r - \delta_v)$ in (C.3).

The value $\delta_v \approx 0.608$ is not allowed for Λ_r , because this value makes the coefficient infinite. According to M11, this value cannot be attained by the range of 4.67 to 6.47 for Λ_r , depending on the values of T_r and p_r . The usual choice of a null standard entropy for dry air and liquid water corresponds to $\Lambda_r \approx L_v / (c_{pd} T) \approx 10$ and to $PV_{s1} \approx PV_e$. The other choice of null standard entropies for dry air and water vapour corresponds to $\Lambda_r = 0$ and to the trivial result $PV_{s1} = PV_\theta$.

Appendix D. An inversion method for PV_{s1} and PV_{q1} : the saturated moist air..

The results obtained in Appendix C for the non-saturated moist air is generalized in this section for the case of a saturated moist air. For the sake of simplicity, the computations will be limited to the description of liquid water content, with the properties $q_v = q_{sw}$ and $q_l = q_t - q_{sw}$. The formulae verified when liquid water is replaced by ice water will be obtained by replacing q_{sw} by q_{si} and L_v by L_s in the next saturated liquid-water PV formulations.

If liquid water content exists, the virtual and moist entropy saturated components (B.5) and (B.6) write

$$PV_v = PV_\theta + \frac{c_{pd}}{3} \delta_v PV(q_t) - \frac{c_{pd}}{3} \left[\frac{\delta_v (1 + \delta)}{\delta} \right] PV(q_l), \quad (\text{D.1})$$

$$PV_{s1} = PV_\theta + \frac{c_{pd}}{3} \Lambda_r PV(q_t) - \frac{c_{pd}}{3} PV\left(\frac{L_v q_l}{c_{pd} T}\right), \quad (\text{D.2})$$

where $\delta_v = \delta (\theta/\theta_v)$.

The differences between the non-saturated and the saturated versions concern only the last PV terms of (D.1) and (D.2), which mainly depend on the gradients of q_l , because the term $q_l PV[L_v(T)/T]$ is *a priori* much smaller than the term $[L_v(T)/T] PV(q_l)$.

The difference between (D.2) and (D.1) generates the water component

$$PV_{q1} = \frac{c_{pd}}{3} (\Lambda_r - \delta_v) PV(q_t) + \frac{c_{pd}}{3} \left[\frac{\delta_v (1 + \delta)}{\delta} \right] PV(q_l) - \frac{c_{pd}}{3} PV\left(\frac{L_v q_l}{c_{pd} T}\right). \quad (\text{D.3})$$

If $\Lambda_r \neq \delta_v$, it is then possible to express $PV(q_t)$ from (D.3) in terms of PV_{q1} plus additional terms mainly depending on the gradients of q_l (if the term depending on $PV[L_v(T)/T]$ is neglected). This expression for $PV(q_t)$ can be replaced in (D.1) and (D.2), leading to the result

$$PV_v = PV_\theta + \left(\frac{\delta_v}{\Lambda_r - \delta_v} \right) PV_{q1} + PV_{l1}, \quad (\text{D.4})$$

where the liquid-water component is equal to

$$PV_{l1} = \frac{c_{pd}}{3} \left(\frac{\delta_v}{\Lambda_r - \delta_v} \right) PV\left(\frac{L_v q_l}{c_{pd} T}\right) - \frac{c_{pd}}{3} \left(\frac{\Lambda_r}{\Lambda_r - \delta_v} \right) \left[\frac{\delta_v (1 + \delta)}{\delta} \right] PV(q_l). \quad (\text{D.5})$$

Comparison of (D.4) with the non-saturated result (C.3) shows that the terms depending on PV_θ and PV_{q1} are the same, except that $\delta_v = \delta / (1 + \delta q_v + q_l)$ depends on q_l . The new liquid-water component PV_{l1} must be added to PV_v which mainly depends on $PV(q_l)$. The non-saturated result is easily obtained if $q_l = 0$, with $\delta_v = \delta / (1 + \delta q_v)$ and with PV_{l1} which exactly cancels out.

An approximate method can be imagined to manage the water component PV_{q1} and the liquid-water component PV_{l1} in (D.4).

The terms depending on q_l might be discarded in the definition (D.3) for PV_{q1} , with accordingly PV_{l1} removed from the saturated result (D.4). The simplified results corresponds to a “just-saturated” moist air version for (D.4). Interestingly, it is the same as the non-saturated system (C.3), with q_v replaced by q_t .

The main advantages of this “just-saturated” assumption is that the same formulation could be used for non-saturated and saturated atmospheric conditions, and that the two components PV_θ and PV_{q1} are probably sufficient for analyzing and modifying PV_v . Additional validations are required to determine whether or not the large scale structures of the liquid-water component PV_{l1} are indeed small correction terms.

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