
Supporting Information for: Non-conservation and conservation for different formulations of moist potential vorticity

Parvathi Kooloth, Leslie M. Smith, Samuel N. Stechmann

Submitted on November 16, 2023
Revised on March 1, 2024

Appendix S1: Thermodynamic variables and conservation

In the main text in section 2.2, several thermodynamic variables are considered (e.g., θ_e and θ_l), and they are commonly assumed to be conserved. Here we add some further descriptions and references for these thermodynamic variables, and we discuss the conservation property that is often assumed for these or other variables.

One thermodynamic variable considered here is the equivalent potential temperature θ_e . Approximate expressions for θ_e that provide intuition for its interpretation are $\theta_e \approx \theta \exp[L_v q_v / (c_{pd} T)]$ and $\theta_e \approx \theta + [L_v \theta / (c_{pd} T)] q_v$, where L_v is the latent heat of vaporization [e.g., 2, 23]. These expressions show that phase changes have two counteracting effects on θ_e , since conversion of vapor q_v to liquid q_l will decrease q_v , while the associated latent heating will increase θ . Accordingly, θ_e is often assumed to be a materially conserved quantity, i.e., $D\theta_e/Dt = 0$.

Another thermodynamic variable considered here is the liquid water potential temperature θ_l . Approximate expressions for θ_l that provide intuition for its interpretation are $\theta_l \approx \theta \exp[-L_v q_l / (c_{pd} T)]$ and $\theta_l \approx \theta - [L_v \theta / (c_{pd} T)] q_l$ [e.g., 2, 23]. These expressions show that phase changes have two counteracting effects on θ_l , since evaporation of liquid q_l will decrease q_l , while the associated evaporative cooling will decrease θ . Accordingly, θ_l is often assumed to be a materially conserved quantity, i.e., $D\theta_l/Dt = 0$.

Note that we have assumed that θ_e and θ_l are conserved quantities, as an approximation that is somewhat common [e.g., 2, 23]. From the perspective of fundamental thermodynamics, though, it is actually a corresponding entropy that is conserved, as follows from the second law of thermodynamics [e.g., 16, 17]. Care must be taken in defining a potential temperature quantity that is related to entropy and is conserved from a fundamental thermodynamics perspective, such as the moist potential temperature quantity θ_s proposed by Marquet [12, 13]. One can also directly define PV in terms of entropy s instead of θ_e or θ_l [e.g., 8]. The important property here for any thermodynamic quantity ψ is whether it is assumed to be materially conserved or not. The presentation here uses θ_e and θ_l as examples because they are perhaps more commonly used than s or θ_s , and they are commonly assumed to be approximately conserved.

Appendix S2: Potential vorticity for Boussinesq systems

For numerical demonstration of the conservation laws from the main text, we set aside the compressible setting that includes acoustic/sound waves and use the simpler setting of the Boussinesq approximation. In this setting, we describe the governing equations and a proof of PV conservation and non-conservation.

Governing Equations

Under the Boussinesq approximation, the governing equations of the moist compressible atmosphere in (1) and (3) of the main text are changed to

$$\frac{D\vec{u}}{Dt} = -\frac{1}{\rho_0}\nabla p' + b'\hat{z}, \quad (1a)$$

$$\frac{D\theta_e}{Dt} = 0, \quad (1b)$$

$$\frac{Dq_t}{Dt} = 0, \quad (1c)$$

$$\nabla \cdot \vec{u} = 0, \quad (1d)$$

where $\vec{x} = (x, y, z)$ is the position vector, $\hat{z}$ is the unit vector in the z -direction, ρ_0 is the constant background density, $\vec{u} = (u, v, w)$ is the velocity, and $D/Dt = \partial/\partial t + \vec{u} \cdot \nabla$ is the material derivative. For similar equations for moist Boussinesq dynamics, see, e.g., [10, 3, 6, 18, 22, 21, 7, 9, 14]. Any thermodynamic variables could be decomposed into a background function of height and an anomalous part, e.g., the equivalent potential temperature $\theta_e(\vec{x}, t) = \tilde{\theta}_e(z) + \theta'_e(\vec{x}, t)$, where $\tilde{\theta}_e(z)$ is prescribed. For liquid water q_l , the background state is zero. Thus p' denotes the pressure anomaly and b' represents the buoyancy, which is, by definition in (4), an anomaly. The total water q_t is the sum of water vapor q_v and liquid water q_l ,

$$q_t = q_v + q_l, \quad (2)$$

and the equivalent potential temperature θ_e is related to the potential temperature θ by

$$\theta_e = \theta + (L/c_p)q_v, \quad (3)$$

where the latent heat L and specific heat c_p are constants with values $L \approx 2.5 \times 10^6 \text{ J kg}^{-1}$ and $c_p \approx 10^3 \text{ J kg}^{-1} \text{ K}^{-1}$. The buoyancy b' may be expressed as

$$b' = g \left(\frac{(\theta - \tilde{\theta}(z))}{\theta_0} + R_{vd}(q_v - \tilde{q}_v(z)) - q_l \right), \quad (4)$$

where R_{vd} is the ratio of gas constants of dry and moist air.

To fully specify (1) in closed form, it is necessary to describe the buoyancy b' in terms of the prognostic variables θ_e and q_t from (1). Hence, we must describe a transformation of variables from (θ_e, q_t) to (θ, q_v, q_l) , as the inverse of the transformation in (2) and (3). To do so, we use different formulas for the transformation, depending on the two possible states of the water content, saturated or unsaturated, and these two states are separated by a phase boundary. The state is determined by comparing the magnitude of the total water specific humidity q_t to the magnitude of a

saturation specific humidity q_{vs} , which acts as a threshold. For simplicity, q_{vs} is approximated by a function of height only such that $q_{vs} \approx q_{vs}(z)$ (see [7] and equation (39) below). This approximation will simplify and facilitate the analytical calculations in (5)–(9), including the formulation of the buoyancy variables in (9), which require consideration of unsaturated versus saturated phases. In unsaturated flow regions with $q_t < q_{vs}$, the water is all in the form of vapor such that $q_t = q_v$, and $q_l = 0$. On the other hand, in saturated regions with $q_t \geq q_{vs}$, then the water vapor is exactly at saturation, and the remaining water is liquid, such that $q_t = q_{vs} + q_l$. Therefore, the formulas for q_v and q_l may be written

$$q_v = \min(q_t, q_{vs}), \quad (5)$$

$$q_l = \max(0, q_t - q_{vs}). \quad (6)$$

Similarly, to recover θ from θ_e and q_t , we write (3) in the unsaturated and saturated phases as $\theta_e = \theta + (L/c_p)q_t$ and $\theta_e = \theta + (L/c_p)q_{vs}$, respectively, and rearrange and combine to arrive at

$$\theta = \theta_e - (L/c_p) \min(q_t, q_{vs}). \quad (7)$$

Together, (5)–(7) show how to write (θ, q_v, q_l) in terms of (θ_e, q_t) , which can be used in (4) to write the buoyancy in terms of the prognostic variables θ_e and q_t .

Furthermore, the presence of phase changes can be made explicit in another way by re-writing the buoyancy b' from (4) as

$$b' = b'_u H_u + b'_s H_s, \quad (8)$$

where the subscript u (s) denotes the unsaturated (saturated) state, H_u, H_s are Heaviside functions and b'_u, b'_s are the expressions for the buoyancies in the different states. More specifically, the Heaviside function $H_u = H(q_{vs} - q_t)$ has the two values $H_u = 1$ for $q_t < q_{vs}$ and $H_u = 0$ for $q_t \geq q_{vs}$, with $H_s = 1 - H_u$. To find the expressions for the buoyancies b'_u and b'_s in terms of the conserved quantities, θ_e and q_t , we insert (5)–(7) into the b' formula in (4). The resulting formulas in the unsaturated and saturated phases are the formulas for b'_u and b'_s :

$$b'_u = g \left(\frac{\theta_e - \bar{\theta}_e(z)}{\theta_0} + \left(R_{vd} - \frac{L_v}{c_p \theta_0} \right) (q_t - \bar{q}_t(z)) \right), \quad b'_s = g \left(\frac{\theta_e - \bar{\theta}_e(z)}{\theta_0} + \left(R_{vd} - \frac{L_v}{c_p \theta_0} + 1 \right) q_{vs}(z) - (q_t - \bar{q}_t(z)) \right). \quad (9)$$

The unsaturated buoyancy b'_u will be used below in defining a potential vorticity variable for illustrating PV conservation and non-conservation. For that purpose, it is necessary to also derive the evolution equations for b'_u and b'_s , which follow from (1b)–(1c) and (9) and have the form [20]

$$\frac{Db'_u}{Dt} + N_u^2 w = 0, \quad \frac{Db'_s}{Dt} + N_s^2 w = 0, \quad (10)$$

where N_u and N_s are the buoyancy frequencies in the unsaturated and saturated regions of the flow, respectively:

$$N_u = \left[g \frac{d}{dz} \left(\frac{\bar{\theta}_e}{\theta_0} + \left(R_{vd} - \frac{L_v}{c_p \theta_0} \right) \bar{q}_t \right) \right]^{1/2}, \quad N_s = \left[g \frac{d}{dz} \left(\frac{\bar{\theta}_e}{\theta_0} - \left(R_{vd} - \frac{L_v}{c_p \theta_0} + 1 \right) q_{vs}(z) - \bar{q}_t \right) \right]^{1/2}. \quad (11)$$

Furthermore, beyond the anomalies b'_u and b'_s , it is helpful to define the associated total quantities b_u and b_s , which

are the total buoyancy in the unsaturated and saturated phases, respectively, defined as

$$b_u = g \left(\frac{\theta_e}{\theta_0} + \left(R_{vd} - \frac{L_v}{c_p \theta_0} \right) q_t \right) = b'_u + N_u^2 z, \quad b_s = g \left(\frac{\theta_e}{\theta_0} - q_t \right) = b'_s + N_s^2 z, \quad (12)$$

These total quantities have evolution equations that follow from (10) and (12) and take the form

$$\frac{D b_u}{D t} = 0, \quad \frac{D b_s}{D t} = 0, \quad (13)$$

so that b_u and b_s are materially conserved. Their material conservation property, and their relationship to the buoyancy, make them interesting candidates for use in defining PV.

Potential Vorticity PV_u

For our numerical study, it is convenient to introduce the moist potential vorticity PV_u based on buoyancy in unsaturated flow regions. As will be discussed, this choice allows us compare material non-conservation (following individual fluid parcels) to volume-integrated conservation (for parcels within a moving material volume).

The moist potential vorticity PV_u is based on the total buoyancy b_u in the unsaturated phase, such that

$$PV_u = \vec{\omega} \cdot \nabla b_u, \quad (14)$$

where b_u is a material invariant, defined in (12) and (13). One could similarly define a moist potential vorticity variable PV_s based on b_s [9], although we focus on PV_u here.

Material Volume-integrated Conservation of PV_u

Derivations of PV conservation laws for the moist Boussinesq equations are as follows. See also [9].

Parcels bounded by surfaces of constant b_u and b_s

We start with the governing equation for PV_u ,

$$\rho \frac{D}{D t} (\vec{\omega} \cdot \nabla b_u) = \nabla b_u \cdot \nabla \times (b' \nabla z). \quad (15)$$

Now we integrate over a material volume that is a distorted cylinder with base and lid given by surfaces of constant b_u (say $b_u = b_{u1}$ and $b_u = b_{u2}$) and sides parametrized as $b_s = b_s(b_u)$:

$$\frac{d}{d t} \iiint_{V_m} dV (\vec{\omega} \cdot \nabla b_u) = \frac{d}{d t} \iiint_{V_a} dV_a J (\vec{\omega} \cdot \nabla b_u) \quad (16)$$

$$= \iiint_{V_a} dV_a \frac{\partial}{\partial t} (\vec{\omega} \cdot \nabla b_u) \quad (17)$$

$$= \iiint_{V_m} dV \rho \frac{D}{D t} (\vec{\omega} \cdot \nabla b_u). \quad (18)$$

The second line results from knowing $J = \frac{\partial(\vec{x})}{\partial(\vec{a})} = \frac{1}{\rho}$ by appropriately choosing $\vec{a}$ is in [19]. And in the moist Boussinesq case, we have $\rho = 1$. Now, using the divergence theorem, since $\nabla b_u \cdot \nabla \times (b' \nabla z) = \nabla \cdot (b_u \nabla \times (b' \nabla z))$, we have,

$$\frac{d}{dt} \iiint_{V_m} dV (\vec{\omega} \cdot \nabla b_u) = \iiint_{V_m} dV \nabla \cdot (b_u \nabla \times (b' \nabla z)), \quad (19)$$

$$= \oint_{S_m} d\vec{S} \cdot b_u \nabla \times (b' \nabla z) = \oint_{S_m} d\vec{S} \cdot (\nabla \times (b' b_u \nabla z) - (b' \nabla b_u \times \nabla z)), \quad (20)$$

$$= - \oint_{S_m} d\vec{S} \cdot (b' \nabla b_u \times \nabla z). \quad (21)$$

On the base and lid, we have $d\vec{S} \parallel \nabla b_u$ i.e., the normal to the surface is parallel to ∇b_u ; as a result, the integrand is zero on the base and the lid, and the integral over the entire surface S_m is the same as the integral over only the sides. Also, if $b_s = b_s(b_u)$ on the sides,

$$- \iint_{S_{sides}} d\vec{S} \cdot (b' \nabla b_u \times \nabla z) = - \iint_{S_{sides}} d\vec{S} \cdot (f(z, b_u) \nabla b_u \times \nabla z) = - \iint_{S_{sides}} d\vec{S} \cdot \nabla \times (g(z, b_u) \nabla z).$$

where $\partial g(b_u, z) / \partial b_u = f(b_u, z)$. Now using Stokes' theorem, we have

$$- \iint_{S_{sides}} d\vec{S} \cdot (b' \nabla b_u \times \nabla z) = - \int_{C_1} d\vec{x} \cdot (g(z, b_u) \nabla z) + \int_{C_2} d\vec{x} \cdot (g(z, b_u) \nabla z) \quad (22)$$

where the curves C_1 and C_2 are the two edges of the distorted cylinder. Finally, note that each of the two curves C_1 and C_2 lies on a surface of constant b_u ; therefore, letting C represent either C_1 or C_2 , the two line integrals above can be evaluated as

$$\int_C d\vec{x} \cdot (g(z) \nabla z) = \int_C d\vec{x} \cdot \nabla G(z) = \int_C dG(z) = 0, \quad (23)$$

where G is an antiderivative of g . This completes the derivation and shows that PV_u , when integrated over a certain material volume V_m , is conserved.

One can also derive the analogous conservation statement for PV_s in a local volume with base and lid as surfaces of constant b_s (say $b_s = b_{s1}$ and $b_s = b_{s2}$) and sides given by $b_u = b_u(b_s)$, by using the same strategy.

Parcels bounded by surfaces of constant θ_θ and q_t

The derivation above can be modified to work for a distorted cylinder with base and lid given by surfaces of constant θ_θ (say $\theta_\theta = \theta_{\theta 1}$ and $\theta_\theta = \theta_{\theta 2}$) and sides parameterized as $q_t = q_t(\theta_\theta)$. Using $\theta_\theta = \theta + \frac{L_v}{c_p} q_v$, b_u can be expressed as a function of θ_θ and q_t . This gives us

$$\nabla b_u = g \left(\frac{1}{\theta_0} \nabla \theta_\theta + \left(R_{vd} - \frac{L_v}{c_p} \right) \nabla q_t \right). \quad (24)$$

Therefore we have,

$$\frac{d}{dt} \iiint_{V_m} dV (\vec{\omega} \cdot \nabla b_u) = - \oint_{S_m} d\vec{S} \cdot \left(b' g \left(\frac{1}{\theta_0} \nabla \theta_e + \left(R_{vd} - \frac{L_v}{c_p} \right) \nabla q_t \right) \times \nabla z \right) \quad (25)$$

$$= - \oint_{S_m} d\vec{S} \cdot \left(b' g \left(\frac{1}{\theta_0} \nabla \theta_e \right) \times \nabla z \right) - \oint_{S_m} d\vec{S} \cdot \left(b' g \left(\left(R_{vd} - \frac{L_v}{c_p} \right) \nabla q_t \right) \times \nabla z \right) \quad (26)$$

$$= I_1 + I_2. \quad (27)$$

For ease of exposition, the first surface integral term with θ_e above will be referred to as I_1 and the latter integral in terms of q_t will be called I_2 . On the base and lid, $d\vec{S} \parallel \nabla \theta_e$ i.e., the normal to the surface is parallel to $\nabla \theta_e$. So, I_1 in the equation above receives zero contribution from integrating over the base and the lid of S_m . Similarly, I_2 receives zero contribution from integrating over the sides of S_m where $q_t = \text{const}$. On the sides, b' can be written as a function of θ_e and z only, therefore

$$I_1 = - \iint_{S_{\text{sides}}} d\vec{S} \cdot \left(b' \frac{g}{\theta_0} \nabla \theta_e \times \nabla z \right) = - \iint_{S_{\text{sides}}} d\vec{S} \cdot (f(z, \theta_e) \nabla \theta_e \times \nabla z) = - \iint_{S_{\text{sides}}} d\vec{S} \cdot \nabla \times (h(z, \theta_e) \nabla z) \quad (28)$$

where $\partial h(\theta_e, z) / \partial \theta_e = f(\theta_e, z)$ and C_1 and C_2 are the top and bottom edges of the cylinder. Now using Stokes' theorem, we have,

$$I_1 = - \int_{C_1} d\vec{x} \cdot (g(z, \theta_e) \nabla z) - \int_{C_2} d\vec{x} \cdot (g(z, \theta_e) \nabla z), \quad (29)$$

where C_1 and C_2 are the top and bottom edges of the cylinder. Note that on C_1 and C_2 , both θ_e and q_t are constants and so,

$$I_1 = - \int_C d\vec{x} \cdot (g(z) \nabla z), \quad (30)$$

$$= - \int_C d\vec{x} \cdot \nabla G(z) = \int_C dG(z) = 0. \quad (31)$$

where $C = C_1 \cup C_2$ and G is an antiderivative of g . Similarly, for I_2 , on the base and the lid where θ_e is constant, b' can be written as a function of only q_t and z . Following the same steps as above, we have

$$I_2 = - \iint_{S_{\text{top/base}}} d\vec{S} \cdot \left(b' g \left(\left(R_{vd} - \frac{L_v}{c_p} \right) \nabla q_t \right) \times \nabla z \right) = - \int_{C_1} d\vec{x} \cdot (h'(z, q_t) \nabla z) - \int_{C_2} d\vec{x} \cdot (h'(z, q_t) \nabla z) \quad (32)$$

and

$$I_2 = \int_C d\vec{x} \cdot (h'(z) \nabla z), \quad (33)$$

$$= \int_C d\vec{x} \cdot \nabla F(z) = \int_C dF(z) = 0. \quad (34)$$

And therefore

$$\frac{d}{dt} \iiint_{V_m} dV (\vec{\omega} \cdot \nabla b_u) = 0, \quad (35)$$

so that volume-integrated PV_u is conserved for material volumes V_m that are distorted cylinders with base and lid given by surfaces of constant θ_e (say $\theta_e = \theta_{e1}$ and $\theta_e = \theta_{e2}$) and sides parameterized as $q_t = q_t(\theta_e)$.

Appendix S3: Further details of numerical simulations

The 3D simulations in this study are performed using the code of [7]. The channel domain has periodic boundary conditions in the x and y directions, and assumes a rigid top and bottom. A third-order Runge-Kutta scheme with adaptive time-stepping (CFL = 0.9) is used for time integration. Spatial discretization is based on pseudo-spectral decomposition using Fourier modes in the horizontal directions, and 2nd-order centered differences on a staggered grid in the vertical direction. In our study, the domain size $L_x \times L_y \times H$ is $8000 \text{ m} \times 8000 \text{ m} \times 7000 \text{ m}$ and the number of grid points is $256 \times 256 \times 400$, corresponding to horizontal and vertical grid spacings of 31.5 m and 17.5 m, respectively.

The flow is confined to the channel by imposing zero vertical velocity w on the top and bottom walls, respectively at $z = H$ and $z = 0$. The horizontal velocities (u, v) are subject to the no-slip condition at the bottom and are allowed to slip at the top. Altogether, (u, v, w) satisfy the top and bottom boundary conditions:

$$w|_{z=0,H} = 0, \quad u|_{z=0} = v|_{z=0} = 0, \quad \frac{\partial u}{\partial z}\bigg|_{z=H} = \frac{\partial v}{\partial z}\bigg|_{z=H} = 0. \quad (36)$$

The anomalous thermodynamic variables $f'(\vec{x}, t)$ obey a homogeneous Neumann boundary conditions on both top and bottom boundaries, such that

$$\frac{\partial f'}{\partial z}\bigg|_{z=0,H} = 0. \quad (37)$$

The code from [7] is adapted to our purpose of testing the inviscid conservation laws by using viscosity and diffusivity coefficients that are very small, with values $O(10^{-15})$. As a comparison, results were compared for viscosity and diffusivity coefficients with values of zero and also values of $O(10^{-15})$ and $O(10^{-9})$, and the differences in PV_u were small and of order of magnitude $O(10^{-15})$ and $O(10^{-9})$, respectively, at measurement time $t = 3 \text{ min}$. Given that the comparisons showed similar results, all results shown here are for the $O(10^{-15})$ case.

The background for the potential temperature θ is idealized to be a linear function of height: $\bar{\theta}(z) = \theta_0 + Bz$, where $\theta_0 = 300 \text{ K}$ and $B = 3 \times 10^{-3} \text{ K m}^{-1}$. Furthermore, we also approximate the saturation specific humidity as that of the background state, $q_{vs}(T, p) \approx q_{vs}(\bar{T}(z), \bar{p}(z)) \equiv q_{vs}(z)$, as also used in the theoretical model description of buoyancy and thermodynamic variables in (4)–(9). In this case, and using an ideal gas law together with the Clausius-Clapeyron relation, the saturation specific humidity $q_{vs}(z)$ may be approximated by

$$q_{vs}(z) = \frac{q_{vs,0}}{\bar{p}(z)/p_0} \exp\left(\frac{-L}{R_v} \left(\frac{1}{h(z)\bar{\theta}(z)} - \frac{1}{\theta_0}\right)\right), \quad (38)$$

where $q_{vs,0} = 20 \text{ g kg}^{-1}$ is the value at $z = 0$, the latent heat $L \approx 2.5 \times 10^6 \text{ J kg}^{-1}$ is constant, and $R_v \approx 462 \text{ kg}^{-1} \text{ K}^{-1}$ is the gas constant for vapor. See Hernandez-Duenas et al. [7] for further details. The background pressure $\bar{p}(z)$ and the function $h(z)$ are given by

$$\frac{\bar{p}(z)}{p_0} = \left(1 - \frac{g}{Bc_p} \log\left(1 + \frac{Bz}{\theta_0}\right)\right)^{c_p/R_d} = [h(z)]^{c_p/R_d}, \quad (39)$$

where the (constant) specific heat is $c_p \approx 10^3 \text{ J kg}^{-1} \text{ K}^{-1}$ and the gas constant for dry air is $R_d \approx 287 \text{ kg}^{-1} \text{ K}^{-1}$. The

background specific humidity $\tilde{q}_v(z)$ is chosen slightly below saturation by using formula (38) with $q_{vs,0}$ replaced by $q_{v,0} = 18 \text{ g kg}^{-1}$.

A rising warm bubble is simulated in the domain to study PV_u conservation in a moist atmosphere. The initial velocity is zero, while the initial anomalies of potential temperature and total water specific humidity are given by, respectively,

$$\theta'(\vec{x}, t = 0) = A_\theta \cos^2 \left(\frac{\pi r(\vec{x})}{2r_c} \right) \quad (40)$$

and

$$q'_t(\vec{x}, t = 0) = A_q \cos \left(\frac{\pi(x - x_c)}{r_c} \right) \cos^2 \left(\frac{\pi r(\vec{x})}{2r_c} \right), \quad (41)$$

where $r(\vec{x}) = \sqrt{(x - x_c)^2 + (y - y_c)^2 + (z - z_c)^2}$, $x_c = L_x/2$, $y_c = L_y/2$, $z_c = 3H/7$, $r_c = 1.5 \text{ km}$, $A_\theta = 2 \text{ K}$ and $A_q = 10^{-3} \text{ kg/kg}$. The form of the potential temperature anomaly is similar to that used in many previous studies of dry thermals [e.g., 11, 4, 1] and moist thermals [e.g., 15]. Some studies have expressed the initial state of the moist thermal in other ways, such as in terms of the relative humidity perturbation [5, 6]. Morrison et al. [15] use a potential temperature perturbation and then define a corresponding water vapor perturbation so that the relative humidity remains the same as the relative humidity of the background state. Here, the initial perturbation of total water in (41) does not bring the state above saturation, so it can be regarded as a perturbation of water vapor. The functional form of (41) is non-spherical due to the $\cos[\pi(x - x_c)/r_c]$ factor. The non-spherical nature of the q'_t anomaly is important for the generation of PV_u . According to (15), PV_u can be generated in the saturated phase, i.e., within a cloud, due to the solenoidal term on the right-hand side. The solenoidal term takes nonzero values when the cross product $\nabla b_u \times \nabla b'$ is nonzero, which can arise, e.g, from having contours of b_u and b' that intersect. Hence, by choosing a spherical perturbation in potential temperature and a non-spherical perturbation in water vapor, the solenoidal term can become nonzero and can generate PV_u inside a cloud.

A material volume V_m can be defined in various ways for the conservation law of material-volume-integrated PV_u . For the numerical simulations, we define V_m to be bounded by surfaces of constant θ_θ and q_t , as an example of the conservation statement from (35). The volume is composed of 29500 grid cells, and at longer evolution times, the volume becomes significantly distorted and stretched. A smaller volume could potentially be distorted and stretched in an even shorter amount of time. Due to distortion and stretching, tracking the volume can potentially become difficult after longer evolution times. Another choice for the material volume could be a ring or torus shape, as a thickened and three-dimensional version of a closed curve, similar to the material curve shown in Figure 4 of the main text.

The simulation in our study is carried out till $t = 4.5 \text{ min}$. For larger times, the simulation becomes numerically unstable as the rising warm bubble nears the top wall. As noted earlier, our numerical method employs very small viscosity and diffusivity coefficients and therefore, cannot handle these wall interactions.

To compare with the plots of PV_u in Figure 2 of the main text, plots of PV_θ are shown in SI Figure S1. One large difference is in the magnitudes of the PV_u versus PV_θ : the maximum value of PV_θ is approximately 100 times larger than that of PV_u . In part this is due to different units, since the definition of buoyancy, in (4) and (9), is proportional to θ but is scaled by a small factor of $g/\theta_0 = (10 \text{ m s}^{-2})/(300 \text{ K}) \approx 0.03 \text{ m s}^{-2} \text{ K}^{-1}$. In part the difference in magnitude is also due to the different PV generation mechanisms for PV_u versus PV_θ : while PV_u is generated by the solenoidal term alone, PV_θ is also generated by cloud latent heating.

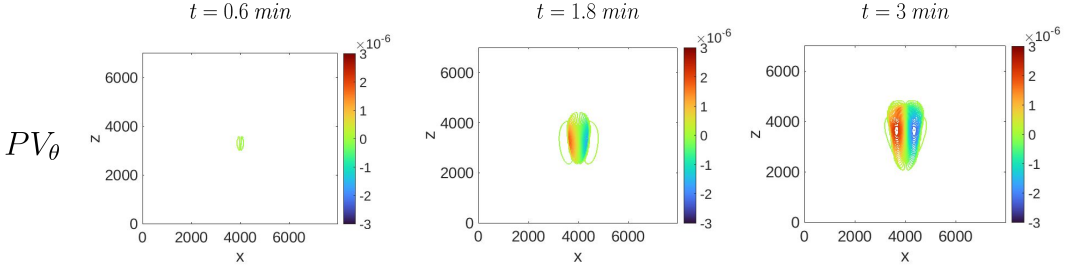


FIGURE S1 Snapshots of PV_θ for the warm bubble in the plane with fixed $y = 0.5L_y = 3500$ m at times $t = 0.6$, 1.8 and 3 minutes. The unit for PV_θ is $\text{K m}^2 \text{kg}^{-1} \text{s}^{-1}$.

146 Appendix S4: Structure of PV_u

In this SI section, we examine the structure of PV_u that is generated in the numerical simulations. To do so, consider the evolution equation of PV_u , which was shown in the main text and is given by

$$\frac{D}{Dt} PV_u = \frac{D}{Dt} (\vec{\omega} \cdot \nabla b_u) = \nabla b_u \cdot (\nabla \times b' \hat{z}). \quad (42)$$

We also noted that the source term goes to zero in the unsaturated phase since $\nabla b_u \cdot (\nabla \times b'_u H_u \hat{z}) = 0$, and therefore PV_u is materially conserved outside a cloud. However, the source term is active in the saturated phase and is given by,

$$\frac{D}{Dt} PV_u = \nabla b_u \cdot (\nabla \times b'_s \hat{z}), \quad \text{if saturated}, \quad (43)$$

which can be rewritten as,

$$\frac{D}{Dt} PV_u = \hat{z} \cdot (\nabla b_u \times \nabla b_s), \quad \text{if saturated}. \quad (44)$$

147 since $b_s - b'_s = N_s^2 z$ and $N_s^2 z$ is only a function of z , and using the cyclic property of scalar triple products. Hence,
 148 it is the z component of the cross-product $(\nabla b_u \times \nabla b_s)$ given by $\partial_x b_u \partial_y b_s - \partial_y b_u \partial_x b_s$ that is responsible of PV_u
 149 generation within the cloud.

150 Now, using equation (44), we can probe the structure of PV_u observed in our simulations. The last panel of the
 151 bottom row of Figure S2 shows the contours of PV_u along $z = 0.5L_z$ plane; a four-lobed structure can be clearly noted.
 152 This four-lobed structure is generated by the z component of $(\nabla b_u \times \nabla b_s)$ as shown in the last panel of the top row
 153 of Figure S2. The zero contours of PV_u are aligned with $x = 4000$ m and $y = 4000$ m along which the gradients of b_u
 154 and b_s are parallel to each other.

155 The bottom panel of Figure S3 and S4 shows that PV_u has a dipole structure along the plane $y = 4000$ m and
 156 $y = 4500$ m. Once again, the dipole structure in PV_u can be understood by considering the term, $\partial_x b_u \partial_y b_s - \partial_y b_u \partial_x b_s$,
 157 in the top panel of Figure S3 and S4. We also note that source term and therefore the resultant PV_u is almost an order
 158 of magnitude larger along $y = 4500$ m as compared to the mid-plane. At the mid-plane, one expects PV_u to be zero, but
 159 non-zero values are present due to the effects of numerical discretization and large gradients across the mid-plane.

160 Based on the plots of PV_u , one can gain some intuition on why PV_u integrates to zero inside specific material

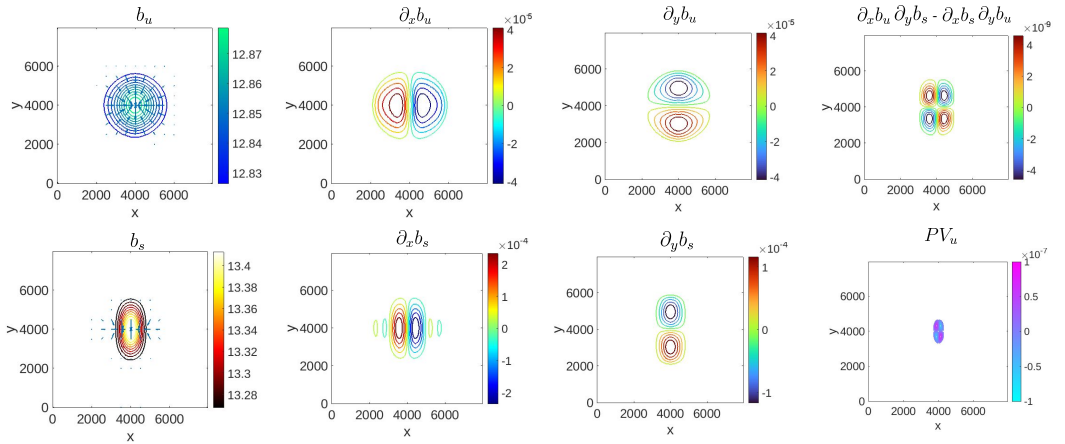


FIGURE S2 Top row: Contour plots along $z = 0.5L_z$ of b_u , $\partial_x b_u$, $\partial_y b_u$ and $\partial_x b_u \partial_y b_s - \partial_x b_s \partial_y b_u$ from left to right. Bottom row: Contour plots along $z = 0.5L_z$ of b_s , $\partial_x b_s$, $\partial_y b_s$ and PV_u from left to right. All plots correspond to $t = 1.2$ min.

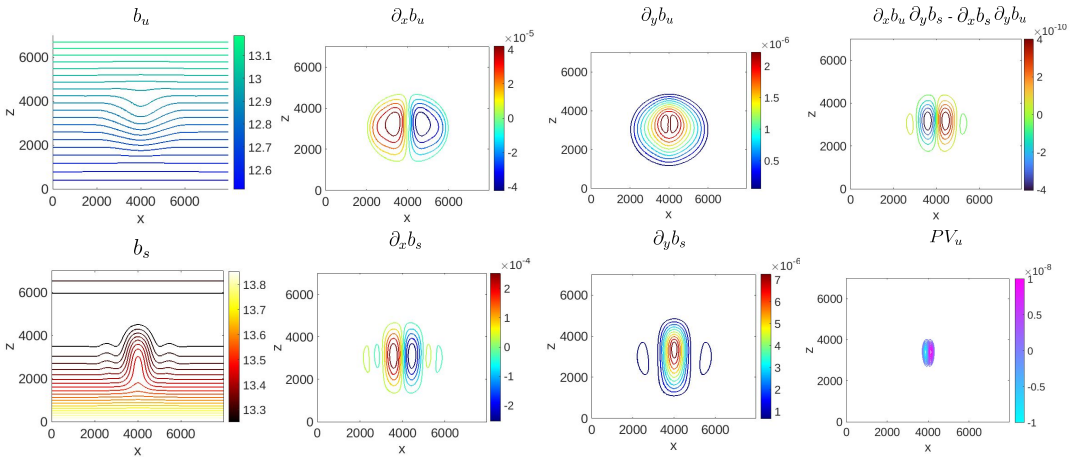


FIGURE S3 Top row: Contour plots along $y = 0.5L_y$ of b_u , $\partial_x b_u$, $\partial_y b_u$ and $\partial_x b_u \partial_y b_s - \partial_y b_u \partial_x b_s$ from left to right. Bottom row: Contour plots along $y = 0.5L_y$ of b_s , $\partial_x b_s$, $\partial_y b_s$ and PV_u from left to right. All plots correspond to $t = 1.2$ min.

161 volumes. The basic idea is that positive and negative anomalies need to be integrated together and cancel each other
 162 exactly. This structure arises from the right-hand side for PV generation, i.e., the solenoidal term, which can be written
 163 in divergence form. Specifically, see (12) and (13) of the main text for a compressible case, and (15) and (16) for the
 164 Boussinesq case of PV_u . The integral of a divergence or derivative is sometimes identically zero, for certain volumes
 165 of integration. One interpretation of this property is that the operation of a divergence or derivative will typically
 166 transform a single local maximum or local minimum into a dipole structure with a positive anomaly accompanied by a
 167 negative anomaly. Also, from the plots of PV_u , one can see that positive anomalies and negative anomalies accompany

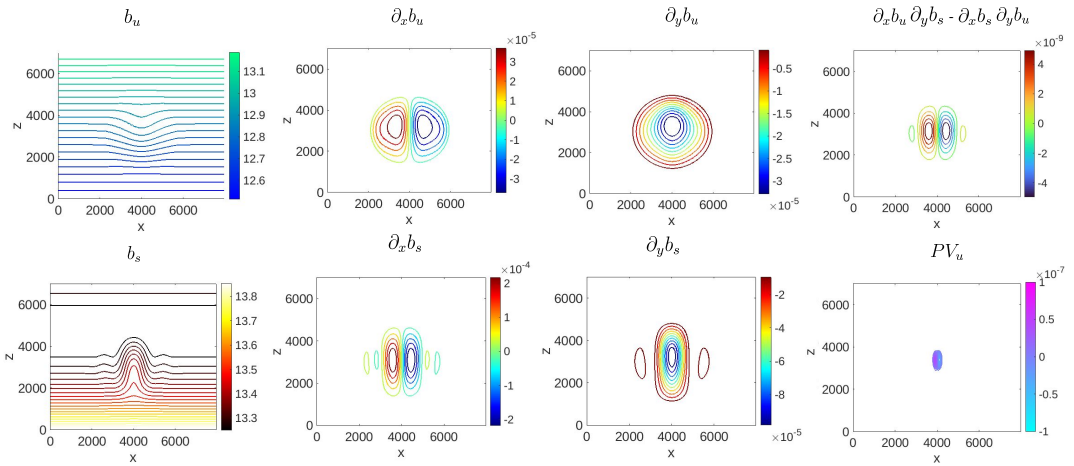


FIGURE S4 Top row: Contour plots along $y = 4500$ m of b_u , $\partial_x b_u$, $\partial_y b_u$ and $\partial_x b_u \partial_y b_s - \partial_x b_s \partial_y b_u$ from left to right. Bottom row: Contour plots along $y = 4500$ m of b_s , $\partial_x b_s$, $\partial_y b_s$ and PV_u from left to right. All plots correspond to $t = 1.2$ min.

each other, due to the form of the solenoidal term for PV generation. For certain material volumes, the positive and negative contributions cancel each other exactly, and lead to volume-integrated PV conservation.

references

- [1] Ahmad, N. and Lindeman, J. (2007) Euler solutions using flux-based wave decomposition. *International Journal for Numerical Methods in Fluids*, **54**, 47–72.
- [2] Betts, A. (1973) Non-precipitating cumulus convection and its parameterization. *Quarterly Journal of the Royal Meteorological Society*, **99**, 178–196.
- [3] Bretherton, C. S. (1987) A theory for nonprecipitating moist convection between two parallel plates. Part I: Thermodynamics and “linear” solutions. *Journal of Atmospheric Sciences*, **44**, 1809–1827.
- [4] Carpenter Jr, R. L., Droegemeier, K. K., Woodward, P. R. and Hane, C. E. (1990) Application of the piecewise parabolic method (PPM) to meteorological modeling. *Monthly Weather Review*, **118**, 586–612.
- [5] Grabowski, W. W. and Clark, T. L. (1991) Cloud–environment interface instability: Rising thermal calculations in two spatial dimensions. *Journal of the Atmospheric Sciences*, **48**, 527–546.
- [6] — (1993) Cloud–environment interface instability: Part II: Extension to three spatial dimensions. *Journal of the Atmospheric Sciences*, **50**, 555–573.
- [7] Hernandez-Duenas, G., Majda, A. J., Smith, L. M. and Stechmann, S. N. (2013) Minimal models for precipitating turbulent convection. *J. Fluid Mech.*, **717**, 576–611.
- [8] Kooloth, P., Smith, L. M. and Stechmann, S. N. (2022) Conservation laws for potential vorticity in a salty ocean or cloudy atmosphere. *Geophysical Research Letters*, **49**, e2022GL100009.
- [9] — (2023) Hamilton’s principle with phase changes and conservation principles for moist potential vorticity. *Quarterly Journal of the Royal Meteorological Society*, **149**, 1056–1072.

-
- [10] Kuo, H. (1961) Convection in conditionally unstable atmosphere. *Tellus*, **13**, 441–459.
- [11] Lilly, D. K. (1962) On the numerical simulation of buoyant convection. *Tellus*, **14**, 148–172.
- [12] Marquet, P. (2011) Definition of a moist entropy potential temperature: Application to FIRE-I data flights. *Quarterly Journal of the Royal Meteorological Society*, **137**, 768–791.
- [13] — (2014) On the definition of a moist-air potential vorticity. *Q. J. Roy. Met. Soc.*, **140**, 917–929.
- [14] Marsico, D. H., Smith, L. M. and Stechmann, S. N. (2019) Energy decompositions for moist Boussinesq and anelastic equations with phase changes. *Journal of the Atmospheric Sciences*, **76**, 3569–3587.
- [15] Morrison, H., Peters, J. M. and Sherwood, S. C. (2021) Comparing growth rates of simulated moist and dry convective thermals. *Journal of the Atmospheric Sciences*, **78**, 797–816.
- [16] Ooyama, K. V. (2001) A dynamic and thermodynamic foundation for modeling the moist atmosphere with parameterized microphysics. *Journal of the Atmospheric Sciences*, **58**, 2073–2102.
- [17] Pauluis, O. (2008) Thermodynamic consistency of the anelastic approximation for a moist atmosphere. *Journal of the Atmospheric Sciences*, **65**, 2719–2729.
- [18] Pauluis, O. and Schumacher, J. (2010) Idealized moist Rayleigh–Bénard convection with piecewise linear equation of state. *Communications in Mathematical Sciences*, **8**, 295–319.
- [19] Salmon, R. (1998) *Lectures on Geophysical Fluid Dynamics*. Oxford University Press.
- [20] Smith, L. M. and Stechmann, S. N. (2017) Precipitating quasigeostrophic equations and potential vorticity inversion with phase changes. *J. Atmos. Sci.*, **74**, 3285–3303.
- [21] Stechmann, S. N. (2014) Multiscale eddy simulation for moist atmospheric convection: Preliminary investigation. *Journal of Computational Physics*, **271**, 99–117.
- [22] Stechmann, S. N. and Stevens, B. (2010) Multiscale models for cumulus cloud dynamics. *Journal of the Atmospheric Sciences*, **67**, 3269–3285.
- [23] Stevens, B. (2005) Atmospheric moist convection. *Annu. Rev. Earth Planet. Sci.*, **33**, 605–643.