



Potential vorticity modification by turbulence in the upper troposphere and lower stratosphere – Part 1: Mechanistic understanding in an upper-level jet-front system

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Abstract. Turbulence has been recognised as an important non-conservative process that modifies potential vorticity (PV) in the upper troposphere and lower stratosphere (UTLS) since the 1970s from research flight measurements. While recent studies based on numerical simulations affirmed the significance of turbulence in changing the PV distribution in the UTLS, the understanding of the underlying mechanism and properties of the PV modification by turbulence remains limited. Therefore, a comprehensive and detailed analysis is required to determine if turbulence may systematically modify PV, which would permit an important up-scale dynamical influence. In this study, we develop an analytical framework and perform a numerical simulation using the Integrated Forecasting System (IFS) model from the European Centre for Medium-Range Weather Forecasts to provide insight into turbulence-induced PV modification. Inspired by the coherent signal near an upper-level jet-front system in the simulation, we first employ an idealised quasi-two-dimensional framework to explore the characteristics of PV modification by turbulence. Both the turbulent heat and the momentum fluxes cause a transfer of PV away from the turbulent zone in most situations, leading to the formation of a tripole pattern of instantaneous PV tendencies. The relevance of the idealised framework to realistic atmospheric flows is validated in the IFS simulation, which features prominent PV tendency tripoles in the frontal zones associated with the upper-level jet stream, consistent with the theory. Material PV changes along air parcel trajectories are further examined by accumulating the instantaneous PV tendencies due to different non-conservative processes in the simulation along the flow. In the vicinity of the upper-level jet-front system, turbulence is shown to be the dominant contributor to accumulated PV changes, which are organised into tripolar bands along the jet axis. By analysing vertical profiles of the atmospheric conditions traced along individual trajectories, air parcels are found to travel consistently through the PV tendency tripoles induced by turbulence. This allows them to steadily accumulate PV changes, which ultimately form the observed tripolar bands. Our results thus (i) provide a mechanistic explanation for the emergence of the tripolar PV tendency pattern due to turbulence with the idealised framework, (ii) demonstrate the possibility of turbulence in systematically modifying PV in the UTLS, which may influence the flow evolution subsequently, and (iii) highlight the importance of the upper-level jet-front systems in providing the spatial and temporal coherence required for the organised behaviour of turbulence in modifying PV. This study therefore advances our understanding of PV modification by turbulence in the UTLS and provides the foundation for future studies, e.g., on the relevance of turbulence to forecast errors and flow dynamics in the UTLS.



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1 Introduction

The importance of diabatic and frictional processes in the dynamics of different extratropical weather systems has been recognised and established by numerous studies in the past decades (see the review by Wernli and Gray, 2024). The potential vorticity (PV) framework (Eliassen and Kleinschmidt, 1957; Hoskins et al., 1985) is often employed when studying synoptic-scale balanced atmospheric flows, as all dynamical information of such flows can be inferred from the distribution of PV with suitable boundary conditions, known as the invertibility principle. PV is defined as (Ertel, 1942):

$$Q = \frac{1}{\rho} (\zeta_a \cdot \nabla \theta), \quad (1)$$

where Q is PV, ρ is density, θ is potential temperature, $\zeta_a = \nabla \times \mathbf{u} + 2\mathbf{\Omega}$ is the absolute vorticity (with $\mathbf{u} = (u, v, w)$ being the velocity and $\mathbf{\Omega}$ the angular velocity of Earth's rotation), and ∇ is the three-dimensional gradient operator in local Cartesian coordinates.

In this framework, the presence of diabatic and frictional processes, including latent heating related to cloud microphysical processes, convection, radiation, and turbulence, precludes the conservation of PV, since the material derivative of PV does not vanish:

$$\frac{DQ}{Dt} = \frac{1}{\rho} (\zeta_a \cdot \nabla \dot{\theta} + \nabla \times \mathbf{F} \cdot \nabla \theta) \quad (2a)$$

$$= -\frac{1}{\rho} \nabla \cdot (-\zeta_a \dot{\theta} + \nabla \theta \times \mathbf{F}), \quad (2b)$$

where $\dot{\theta}$ is the diabatic heating rate, and $\mathbf{F}$ is the non-conservative force. Note that though the operands of the divergence operator in Eq. (2b) (i.e., $-\zeta_a \dot{\theta} + \nabla \theta \times \mathbf{F}$) are referred to as the “non-advective flux of PV substance” (Haynes and McIntyre, 1987, 1990), we utilise the (technically imprecise) term “non-advective PV flux” hereafter for brevity. As shown in Eq. (2b), a convergence of the non-advective PV flux will lead to a material increase of PV. Therefore, diabatic and frictional processes, which induce non-advective PV flux, may cause material changes of PV and induce far-field effects that alter the evolution of the larger-scale flow. The PV modification by these non-conservative processes may thus be used to indicate and quantify their influence on the flow evolution.

In particular, PV modification in the upper troposphere and lower stratosphere (UTLS) deserves attention, since it is highly relevant for the synoptic-scale dynamics in the mid-latitudes. For instance, diabatic processes are found to induce prominent PV modification across the tropopause (Chagnon et al., 2013; Chagnon and Gray, 2015), which influences the nonlinear evolution of Rossby waves. The phase speed of Rossby wave is also dependent on the isentropic PV gradient (Harvey et al., 2016), which could be modified by non-conservative processes significantly near the tropopause (Saffin et al., 2017). Moreover, if one adopts the concept of a dynamical tropopause, which is usually defined as an isosurface of PV (2 PVU is used in this study, where 1 PVU = $1 \times 10^{-6} \text{ K kg}^{-1} \text{ m}^2 \text{ s}^{-1}$), non-conservative processes are required for stratosphere-troposphere exchange (STE; Stohl et al., 2003). While radiation and turbulence were first considered as relevant processes for STE (e.g., Staley, 1960; Shapiro,



1976, 1980), later studies also revealed the importance of latent heating related to cloud processes and convection (e.g., Price and Vaughan, 1993; Lamarque and Hess, 1994; Gray, 2006).

With further improvements in numerical models and refinements in methodology, recent studies that attributed PV modification to individual processes consistently demonstrated the significant role of turbulence in the UTLS. In their systematic evaluation of PV modification in Rossby waves using the Met Office Unified Model, Saffin et al. (2017) found that turbulent mixing in the UTLS induces a systematic dipole PV modification that sharpens the tropopause. Turbulence was shown to contribute the largest and second largest PV changes in ridges and troughs, respectively, among all the parametrised non-conservative processes (Saffin et al., 2017, their Fig. 3c). On the other hand, Spreitzer et al. (2019) studied the PV modification in the European Centre for Medium-Range Weather Forecasts (ECMWF) model using tendency diagnostics. They showed that turbulence is responsible for generating the positive PV anomaly on the stratospheric side of the upper-level jet, for the decay of the tropopause fold, and for the formation of a vertical tripole of PV modification (positive-negative-positive) at the elevated tropopause in the ridge. These two studies clearly illustrated that turbulence can induce coherent material PV changes, making it relevant to the dynamics in the UTLS.

Although turbulence was shown to be capable of causing dynamically relevant PV changes in the UTLS, the mechanism or pathway through which turbulence achieves such PV modification is much less explored and understood. Conceptually, to generate coherent material PV changes, there are at least two layers of complexity. First, the turbulence-induced instantaneous PV tendencies have to be structured or spatially coherent. If the PV tendency field was random and chaotic, there would be hardly any systematic PV modification as time progresses. Second, the accumulation of PV tendencies, which leads to the resultant material PV changes, has to be organised or coherent in time as well. A certain arrangement of the flow and PV tendencies is likely required for the emergence of the reported PV modification signal due to turbulence.

While clear signals of PV modification by turbulence were shown in Saffin et al. (2017), there is no explanation for the formation of that dipole pattern of PV changes. Spreitzer et al. (2019) linked the formation of the spatial patterns of PV tendencies observed to the turbulent heating profile, following Shapiro (1976). Though this is plausible for the existence of the positive PV anomaly on the stratospheric side of the jet, the tripole patterns found in other regions have a clear contribution from the turbulent momentum transfer (Spreitzer et al., 2019, their Fig. 6a), which is not considered in the original explanation by Shapiro (1976). The combined effects of turbulent heat and momentum transfer were studied in early numerical studies (Gidel and Shapiro, 1979; Hartjenstein, 2000), which were based on simplified two-dimensional isentropic models. Although the result of Hartjenstein (2000) also displayed a tripole pattern that closely resembles those observed by Spreitzer et al. (2019), whether this is a coincidence or a systematic behaviour of PV modification by turbulence remains unclear, since it lacks the support from an analytical description.

Consequently, a comprehensive understanding of PV modification by turbulence in the UTLS is best achieved by combining an analysis of the governing equations and a verification of the results obtained in a three-dimensional numerical model that can simulate realistic atmospheric flows. Therefore, in this study, we revisit the equations and introduce a simplified framework to describe the characteristics of PV modification by turbulence in the UTLS. We also utilise a simulation performed with the



90 Integrated Forecasting System (IFS) from ECMWF to inspire and verify the analytical framework. With both tools, we would like to advance our understanding of the following specific research questions:

1. How does turbulence modify PV instantaneously? Is there a systematic or coherent behaviour?
2. Are there coherent material PV changes formed through the accumulation of instantaneous PV tendency due to turbulence? How do they arise?

95 In this first part of our study, we focus on an upper-level jet-front system in the simulation because turbulence occurs frequently in the neighbourhood of such systems (e.g., Bannon, 1952; Koch et al., 2005; Rodriguez Imazio et al., 2022). It also suits the illustration of the concepts developed in and facilitates the comparison with previous studies analysing the same type of flow system (e.g., Shapiro, 1976; Gidel and Shapiro, 1979; Hartjensstein, 2000). A more complex flow situation will be explored in the second part of this study.

100 The remaining parts of this paper are structured as follows. The data and methods are introduced in Sect. 2, followed by the outline of the idealised analytical framework in Sect. 3. The characteristics of PV modification by turbulence derived from the framework are presented in Sect. 4 and their representation in the IFS simulation is examined in Sect. 5. The accumulation of PV changes due to turbulence in time is explored in Sect. 6, followed by a discussion on other interesting aspects of the results in Sect. 7. The major conclusions are then summarised in Sect. 8.

105 **2 Data and methods**

To address the research questions, we conduct a dedicated simulation using the IFS, the operational numerical weather forecasting model at ECMWF (Sect. 2.1). From the simulation, we output temperature and momentum tendencies from each parametrised non-conservative process, allowing us to directly examine the simulated PV tendencies induced by turbulence and other parametrised processes (Sect. 2.2). To go beyond a single case study, we use the simulation results as an inspiration,
110 upon which we develop an idealised framework to better understand the systematic characteristics of turbulence-induced PV modification in general. The validity of the idealised framework in realistic atmospheric flows is then assessed in the simulation by checking the consistency between them. To evaluate how coherent material PV changes are formed, we perform a Lagrangian analysis (Sect. 2.3), complementing the instantaneous Eulerian view. The results obtained with these different tools will provide us a more nuanced understanding of the PV modification by turbulence in the UTLS.

115 **2.1 The IFS simulation**

The dedicated IFS simulation plays a central role in this study. The IFS is a coupled model for the Earth system and is used to generate operational weather forecasts at ECMWF. The model version of IFS used in this study is Cy47r3, which was the operational version at ECMWF from October 2021 to June 2023. It has a major update in moist physics compared to its predecessors (Bechtold et al., 2020; Forbes et al., 2021). The simulations are run with a triangular-cubic-octahedral spectral
120 transform discretisation of TCo1279, which corresponds to a horizontal resolution of approximately 9 km. In the vertical



direction, there are 137 terrain-following sigma-hybrid model levels, with a resolution of around 300 m near the extratropical tropopause. The model has an internal time step of 7.5 minutes and the fields are output at hourly intervals. The outputs from the simulations are horizontally interpolated to a regular latitude-longitude grid with 0.1° resolution and used in the subsequent analysis.

125 Non-conservative processes, including turbulence, usually act at scales smaller than the resolved scales and their effects are represented in the IFS via different physical parametrisation schemes. To examine their influence on PV modification, we output the instantaneous temperature and momentum tendencies from individual parametrisation schemes, similar to Spreitzer et al. (2019); Attinger et al. (2019, 2021); Volonté et al. (2025). For the application in this study, these non-conservative processes are separated into five groups, namely shortwave radiation, longwave radiation, convection, cloud processes, and
130 turbulence. The parametrisations are called sequentially to update the prognostic variables at the grid scale, which makes the temperature and momentum tendencies, i.e., $\dot{T}_i$ and $\mathbf{F}_i = (\dot{u}_i, \dot{v}_i, 0)$ from each process additive and their sum gives the total tendencies $\dot{T}$ and $\mathbf{F}$ due to all these processes ($\dot{u}_i$ denotes the eastward and $\dot{v}_i$ the northward wind tendency; there is no vertical wind tendency due to parametrisations in the IFS).

While a detailed documentation of the implementation can be found in ECMWF (2021), we here describe briefly the
135 parametrisations of processes that we grouped into the category “turbulence”. The turbulent diffusion scheme in the IFS represents the vertical mixing of heat, momentum, and moisture due to subgrid-scale turbulence. The turbulent fluxes in the outer layer (i.e., exchange between model levels) are modelled using a K-diffusion closure except in the mixed layer of an unstable boundary layer, where the eddy-diffusivity mass-flux approach (Köhler et al., 2011) is applied to represent non-local mixing.

Since the UTLS is mostly outside of the mixed layer, turbulent transport there is modelled using the K-diffusion closure with
140 the exchange coefficients given by the Monin-Obukhov similarity theory in statically stable layers and by the revised Louis scheme (Louis et al., 1982) in statically unstable layers. While these exchange coefficients are functions of the local Richardson number, vertical wind shear, and other quantities like mixing length, the turbulent diffusion scheme remains in the form of the flux-gradient theory or the K-theory (Holton and Hakim, 2013). Finally, a dissipation of kinetic energy into internal energy is included to close the energy cycle. In addition, parametrisations to account for the momentum transport of turbulent orographic
145 form drag (Beljaars et al., 2004), blocked-flow drag, orographic gravity wave drag (Lott and Miller, 1997), and non-orography gravity wave drag (Orr et al., 2010) are also assigned to the turbulence category and aggregated into the temperature tendency $\dot{T}_{turb}$ and the momentum tendencies $\mathbf{F}_{turb} = (\dot{u}_{turb}, \dot{v}_{turb}, 0)$ due to turbulence (denoted by the subscript “turb”). While the turbulence term technically contains contributions from flow drag, the major signals near the tropopause appear to be caused by turbulent diffusion, which is the focus of this study.

150 2.2 Instantaneous PV tendency derived from model output

In this paper, we examine the results from one simulated case that is initialised from the analysis at 12 UTC on 29 August 2019. We choose to analyse the atmospheric fields with a 24 h forecast lead time (valid at 12 UTC on 30 August 2019) as it allows the investigation of the short-term evolution of the flow while minimising forecast errors. The region of interest is the North Atlantic basin and the PV fields at 200 and 350 hPa are shown in Fig. 1a and b, respectively. A synoptic-scale PV

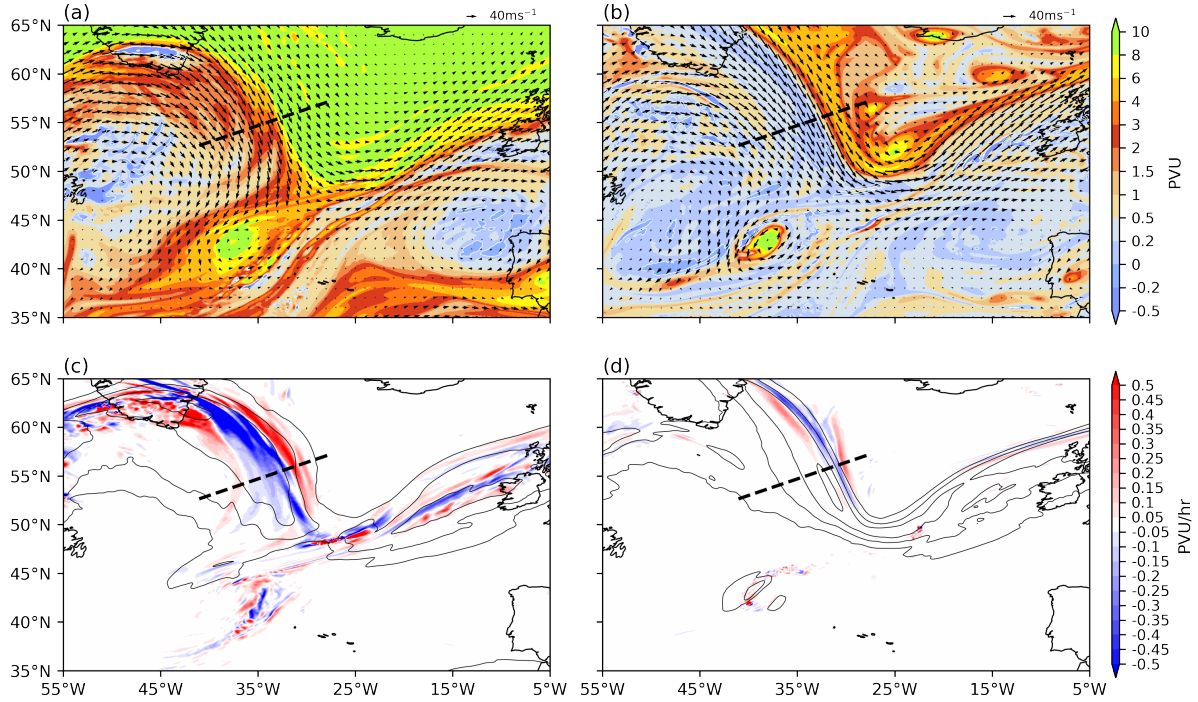


Figure 1. (a,b) PV and (c,d) instantaneous PV tendency due to turbulence at (a,c) 200 hPa and (b,d) 350 hPa at 12 UTC on 30 August 2019 of the dedicated IFS simulation. Wind vectors (black arrows) are overlaid in (a,b) while isotachs are overlaid in (c,d) starting from 30 m s^{-1} at 10 m s^{-1} intervals. The black dashed line indicates the location of the vertical cross section examined in Sect. 5.

155 trough is present over the North Atlantic with a stratospheric PV cutoff ($> 2 \text{ PVU}$) detaching from its southern tip. The high wind speeds found on both the upstream and downstream flanks of the trough indicate a meandering upper-level jet stream. On the upstream flank of the trough, a narrow tongue of stratospheric air is present at 350 hPa (Fig. 1b), which is part of the tropopause fold or the upper-level front (more details in Sect. 5). The neighbourhood of this upper-level jet-front system also exhibits enhanced vertical wind shear (not shown), which likely activates the turbulent diffusion parametrisation in the model.

160 From the hourly archived instantaneous temperature tendencies $\dot{T}_i$ and momentum tendencies $\mathbf{F}_i = (\dot{u}_i, \dot{v}_i, 0)$ of each process i we derive instantaneous PV tendencies. First, $\dot{T}_i$ is converted to a potential temperature tendency $\dot{\theta}_i$ for each diabatic process according to:

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

where p is pressure, $p_0 = 1000 \text{ hPa}$, and $\kappa = 0.286$. With both $\dot{\theta}_i$ and $\mathbf{F}_i$, the PV tendency of process i can then be obtained from Eq. (2), as the equation is linear to both $\dot{\theta}$ and $\mathbf{F}$. The total PV tendency due to all non-conservative processes is thus just the sum of the contributions from all the processes.



Figures 1c and d display the PV tendency due to turbulence on 200 and 350 hPa, respectively, at 12 UTC on 30 August 2019. In the vicinity of the upper-level jet-front system, prominent PV tendency signals are generated by the turbulence parametrisation scheme at both isobaric levels. In particular, elongated bands of alternating signs are found in the turbulence-induced PV tendency field that roughly align with the jet axis. These coherent signals associated with the upper-level jet-front system serve as the first indication of a possibly systematic behaviour of PV modification by turbulence in the UTLS. These elongated bands will be analysed further in later sections. More localised spots of high PV tendencies can be observed on the southeastern sides of the stratospheric PV cutoff and the PV trough or near the tip of the upstream ridge. While only the upper-level jet-front system will be discussed in this paper, other interesting features in these PV tendency fields were discussed in Lee (2025).

2.3 Lagrangian analysis

To address the second research question, which concerns the material PV change, we run backward trajectories and analyse the Lagrangian history of different air parcels. The method used is based on reverse domain filling, which allows the examination of the origin of air parcels or tracers by computing backward trajectories. This method has long been used in previous research (e.g., Sutton et al., 1994; Schoeberl and Newman, 1995; Liniger and Davies, 2003) and later to study PV modification by non-conservative processes (e.g., Joos and Wernli, 2012; Chagnon et al., 2013; Crezee et al., 2017; Spreitzer et al., 2019; Attinger et al., 2019).

The material PV change ΔQ equals the integration of the instantaneous PV tendency $\frac{DQ}{Dt}$ along the backward trajectory of an air parcel $\mathbf{x}(t)$:

$$\Delta Q(\mathbf{x}(t_0), t) = Q(\mathbf{x}(t_0), t_0) - Q(\mathbf{x}(t), t) = \int_t^{t_0} \frac{DQ(\mathbf{x}(\tau), \tau)}{Dt} d\tau, \quad (4)$$

with $t < t_0$ for backward trajectories.

From Eq. (4), one may obtain ΔQ in two different ways. First, once the backward trajectory is computed, the PV values of an air parcel at time t and t_0 can be extracted, which allows the computation of $Q(\mathbf{x}(t_0), t_0) - Q(\mathbf{x}(t), t)$ and hence ΔQ . $Q(\mathbf{x}(t), t)$ can also be thought of as the PV advected to location $\mathbf{x}(t_0)$ conservatively from t to t_0 (Q_{adv}), i.e.,

$$Q_{\text{adv}}(\mathbf{x}(t_0), t) = Q(\mathbf{x}(t), t). \quad (5)$$

Second, one may obtain ΔQ by tracing the PV tendencies experienced by the air parcel along the trajectory and get the accumulated PV change during the interval from time t to t_0 by computing the integral on the right of Eq. (4). Since model outputs have a finite time step Δt in practice, this integration is discretised and approximated by a summation. The total accumulated PV change (APV) from time step t_n to t_0 is hence given by:

$$\text{APV}(\mathbf{x}(t_0), t_n) = \sum_{k=0}^{n-1} \left(\frac{DQ(\mathbf{x}(t_k), t_k)}{Dt} \right) \Delta t, \quad (6)$$

with $t_k = t_0 - k\Delta t$. The PV tendency at time t_n is not included as the tendency at each time step is used to represent the situation over the previous hour. With this approximation made, a residue exists between APV and ΔQ due to the discretisation



error. However, the computation of APV has a benefit as it allows a further partition into the contributions from the individual non-conservative processes. One may separate APV into contributions by each process i :

$$\text{APV} = \sum_i \text{APV}_i = \sum_i \sum_{k=0}^{n-1} \left(\frac{DQ(\mathbf{x}(t_k), t_k)}{Dt} \right)_i \Delta t. \quad (7)$$

200 Therefore, in practice:

$$\Delta Q(\mathbf{x}(t_0), t) = Q(\mathbf{x}(t_0), t) - Q_{\text{adv}}(\mathbf{x}(t_0), t) = \sum_i \text{APV}_i + \text{residue}. \quad (8)$$

In this study, ΔQ in the UTLS region is investigated by initialising backward trajectories at every grid point (0.1° regular grid for the dedicated IFS simulation) on isobaric surfaces with a 25 hPa interval. The trajectories are calculated with LAGRANTO (Sprenger and Wernli, 2015), with hourly wind fields from the IFS output. They are computed up to 18 h backwards in time in order to focus on the most recent changes. The backward trajectories are utilised to estimate ΔQ in the two ways mentioned above. We note that both estimates are subject to interpolation errors due to offline trajectory calculation. Also, while ΔQ estimated from Q_{adv} is our best approximation to the true value and will be used to represent the material PV change in the IFS simulation, it can still contain errors due to numerical diffusion of the dynamical core.

As a quick tool to assess the relative importance of the processes in causing the ΔQ observed, we develop a simple method to attribute to each air parcel its dominant PV-modifying process. If ΔQ is positive, the dominant cause is attributed to the largest positive contribution from terms among APV_i and the residue (Eq. 8), and analogously if ΔQ is negative. The inclusion of the residue in the comparison is to account for the uncertainty due to discretisation errors. If the residue is large and exceeds the contribution by any individual process, a major part of ΔQ is not captured by the integrated PV tendencies and its cause is deemed uncertain.

215 3 An idealised quasi-two-dimensional framework for PV modification by turbulence

As outlined in Sect. 2, we attempt to understand the formation of coherent patterns of PV tendencies due to turbulence by adopting an idealised framework, which allows an easier interpretation given the simplifications made. To build such a framework, we first adopt the flux-gradient approach (or the K-theory) to describe the effect of turbulence in the vertical (Sect. 3.1), as is typically done regarding atmospheric flow. Furthermore, inspired by the elongated features observed, we simplify the situation by considering only variations and the resulting PV tendencies in a two-dimensional vertical cross section (Sect. 3.2).

3.1 Flux-gradient theory for turbulent fluxes

Turbulence near the tropopause is unarguably initiating both heat and momentum transfer in the UTLS, but it is difficult to capture the effect of each turbulent eddy. A simple way to describe the overall effect is the flux-gradient theory, in which the turbulent eddy fluxes are assumed to be proportional to the local gradients of the mean flow (Holton and Hakim, 2013), analogous to molecular diffusion. In atmospheric flows, the vertical gradients are usually larger in magnitude compared to the



horizontal gradients and therefore more important. In the flux-gradient theory, the turbulent heat and momentum fluxes in the vertical direction are modelled respectively as follows:

$$\overline{\theta'w'} = -K_h \frac{\partial \bar{\theta}}{\partial z} \quad (9a)$$

$$\overline{u'w'} = -K_m \frac{\partial \bar{u}}{\partial z} \quad (9b)$$

$$230 \quad \overline{v'w'} = -K_m \frac{\partial \bar{v}}{\partial z}, \quad (9c)$$

where K_h is the eddy diffusivity of heat, K_m is the eddy viscosity coefficient, and quantities with an overbar are Reynolds averaged means while primed quantities are the corresponding deviations. Since the mean quantities like $\bar{\theta}$ can also be interpreted as quantities that represent the resolved scales, the overbars will be dropped in the following sections for simplicity.

While the simplest model would assume constant K_h and K_m , one can also treat these exchange coefficients as functions of vertical wind shear and static stability, as is done in the free atmosphere in the IFS (ECMWF, 2021). High wind shear tends to enhance turbulence while strong static stability tends to suppress it. Turbulence is hence usually modelled to be strong in regions with strong vertical wind shear, for instance in the regions above and below the upper-level jet core.

According to the flux-gradient theory, the tendencies of potential temperature and momentum depend on the vertical convergence of the corresponding turbulent flux:

$$240 \quad \dot{\theta}_{turb} = -\frac{1}{\rho} \frac{\partial \rho \overline{\theta'w'}}{\partial z} \quad (10a)$$

$$\dot{u}_{turb} = -\frac{1}{\rho} \frac{\partial \rho \overline{u'w'}}{\partial z} \quad (10b)$$

$$\dot{v}_{turb} = -\frac{1}{\rho} \frac{\partial \rho \overline{v'w'}}{\partial z}. \quad (10c)$$

Therefore, with Eq. (9) and (10), the tendencies due to turbulence can be worked out from the corresponding background gradients in the vertical profile (assuming the variation in density is less significant than that of the turbulent fluxes).

3.2 Quasi-two-dimensional approximation

We now proceed to examine the effect of turbulence on PV in idealised settings. While PV tendencies, as seen in Eq. (2), result from the three-dimensional variations of the tendencies of potential temperature and horizontal winds, the elongated structures observed in Fig. 1 suggest that there exists a certain horizontal direction along which the variations are smaller, making the system quasi-two-dimensional (invariant when translated along this direction). Therefore, we simplify the situation by restricting the discussion to a vertical cross section in the yz plane, with the x -axis aligned with the direction of small variation. For easier reference, this direction is referred to as the “coherent direction” in the following. With this coordinate system, the notations (u, v) and $(\dot{u}, \dot{v})$ no longer indicate winds or momentum tendencies in the absolute eastward and northward directions, but perpendicular and along the considered two-dimensional section, respectively.

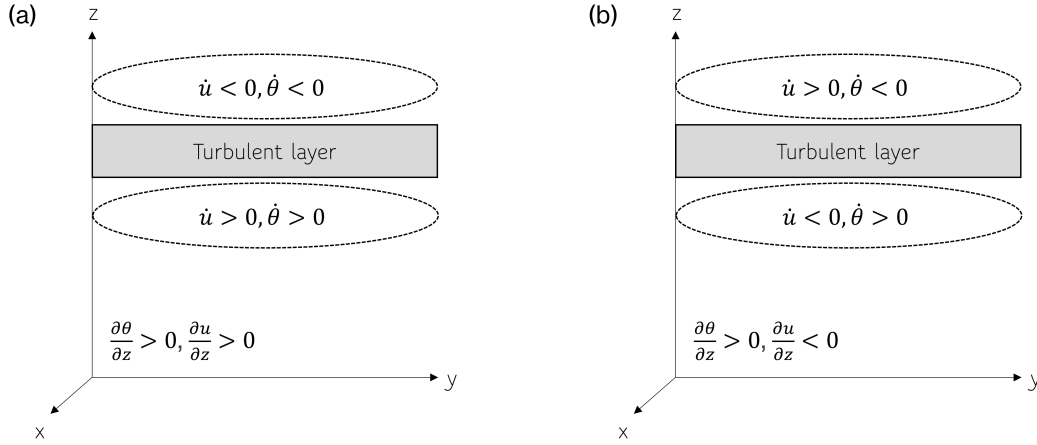


Figure 2. Schematics of potential temperature and momentum tendency dipoles induced by a turbulent layer in a vertical cross section. Turbulent fluxes have maximum magnitudes within the grey shaded layer. In both situations (a) and (b), θ is increasing with height, while u is increasing with height in (a) and decreasing in (b). The configuration in (a) resembles the region below the jet core and that in (b) the region above the jet core. The signs of the potential temperature and momentum tendency dipoles are indicated for the corresponding regions.

255 Consider an idealised situation in which a horizontal layer of finite depth with strong turbulence is present in this yz plane and hence a local maximum in the turbulent flux profile, as shown schematically in Fig. 2. Here θ is assumed to be increasing with height, as the atmosphere is generally statically stable. In Fig. 2a, since the background gradients of θ and u point upward, the turbulent heat and momentum fluxes point downward (see Eq. 9). With the maximum flux at the height of the turbulent layer, the layer above will have a divergence of heat and momentum fluxes, which decreases θ and u in this layer (see Eq. 10).
260 The layer below will instead have a convergence of the fluxes and increasing θ and u . In contrast, if the background gradient of u points downward, flux convergence is found above and divergence below, as shown in Fig. 2b.

Consequently, positive and negative pairs of tendencies of potential temperature ($\dot{\theta}$) and momentum ($\dot{u}$) are generated and form a dipole pattern across the turbulent layer. This holds both in situations with the vertical wind shear and potential temperature gradient having the same (Fig. 2a) and opposite (Fig. 2b) directions, corresponding to the conditions below and above
265 the upper-level jet core, respectively.

These tendencies induced by turbulence modify PV according to Eq. (2b). However, with the quasi-two-dimensional approximation, we may assume $\frac{\partial}{\partial x}(\dots) \ll \frac{\partial}{\partial y}(\dots)$. Together with scale analysis, Eq. (2b) reduces to (see Appendix A for the full derivation):

$$\begin{aligned} \frac{DQ}{Dt} &\simeq \frac{1}{\rho} \left\{ -\frac{\partial}{\partial y} \left(-\dot{\theta} \frac{\partial u}{\partial z} + \dot{u} \frac{\partial \theta}{\partial z} \right) - \frac{\partial}{\partial z} \left[\dot{\theta} \left(\frac{\partial u}{\partial y} - f \right) - \dot{u} \frac{\partial \theta}{\partial y} \right] \right\} \\ &= \frac{1}{\rho} \left[-\frac{\partial}{\partial y} \left(\underbrace{-\dot{\theta} \frac{\partial u}{\partial z}}_1 + \underbrace{\dot{u} \frac{\partial \theta}{\partial z}}_2 \right) - \frac{\partial}{\partial z} \left(\underbrace{\dot{\theta} \frac{\partial u}{\partial y}}_3 - \underbrace{\dot{u} \frac{\partial \theta}{\partial y}}_4 \right) \right], \end{aligned} \quad (11)$$



270 where we introduce the absolute momentum $m = u - fy$ in this cross section (f is the Coriolis parameter), which can be interpreted as the Cartesian analogy to the absolute angular momentum for the rotating Earth (Keyser and Shapiro, 1986).

To inspect the physical meaning of the terms in Eq. (11) and their relations to Eq. (2b), we express Q and ζ_a in the yz plane and introduce the two-dimensional vectors $\mathbf{H}$ and $\mathbf{M}$:

$$Q = \frac{1}{\rho} (\zeta_a \cdot \nabla \theta) = \frac{1}{\rho} \left(\frac{\partial \theta}{\partial y} \frac{\partial m}{\partial z} - \frac{\partial \theta}{\partial z} \frac{\partial m}{\partial y} \right) \quad (12a)$$

$$275 \quad \zeta_a = -\hat{\mathbf{i}} \times \nabla m = \left(\frac{\partial m}{\partial z} \right) \hat{\mathbf{j}} - \left(\frac{\partial m}{\partial y} \right) \hat{\mathbf{k}} \quad (12b)$$

$$\mathbf{H} = \dot{\theta} (\hat{\mathbf{i}} \times \nabla m) = -\dot{\theta} \left(\frac{\partial m}{\partial z} \right) \hat{\mathbf{j}} + \dot{\theta} \left(\frac{\partial m}{\partial y} \right) \hat{\mathbf{k}} \quad (12c)$$

$$\mathbf{M} = -\dot{u} (\hat{\mathbf{i}} \times \nabla \theta) = \dot{u} \left(\frac{\partial \theta}{\partial z} \right) \hat{\mathbf{j}} - \dot{u} \left(\frac{\partial \theta}{\partial y} \right) \hat{\mathbf{k}}. \quad (12d)$$

From Eq. (12b), it is clear that ζ_a is parallel to constant m surfaces ($\zeta_a \cdot \nabla m = 0$) and pointing to the right of ∇m in the yz plane. In this two-dimensional framework, the $\mathbf{H}$ vector is equivalent to $-\zeta_a \dot{\theta}$ and corresponds to terms 1 and 3 in Eq. (11). It is therefore the heat transfer term and acts along constant m surfaces in the yz plane. Similarly, the $\mathbf{M}$ vector is related to the momentum transfer term $\nabla \theta \times \mathbf{F}$ and corresponds to terms 2 and 4 in Eq. (11). From its mathematical form, $\mathbf{M}$ acts along isentropic surfaces in the yz plane, which also holds for its three-dimensional equivalent. Also, with these new notations, we can rewrite Eq. (11) elegantly as:

$$285 \quad \frac{DQ}{Dt} = -\frac{1}{\rho} \nabla \cdot (\mathbf{H} + \mathbf{M}), \quad (13)$$

with $\nabla \cdot$ here referring to the two-dimensional divergence operator in the yz plane. Equation (13) shows that the PV tendency is proportional to the convergence of the vector field $\mathbf{H} + \mathbf{M}$ in the yz plane. The vectors $\mathbf{H}$ and $\mathbf{M}$ therefore represent the non-advective PV fluxes in this two-dimensional framework.

To summarise, the idealised framework consists of two fundamental assumptions: (i) the flux-gradient theory can be used to describe the effect of turbulence in the UTLS; and (ii) there exists a coherent direction, along which the quasi-two-dimensional approximation can be justified. With the flux-gradient theory, the heat and momentum tendencies due to turbulence above or below a turbulent layer can be derived from the corresponding background gradients. The resulting PV tendencies can then be approximated by Eq. (11), provided that the system is quasi-two-dimensional. The introduction of the vectors $\mathbf{H}$ and $\mathbf{M}$ is insightful to examine the characteristics of PV modification by turbulence due to heat and momentum fluxes in this two-dimensional framework, as explained in the next section.



4 Characteristics of PV modification by turbulence

4.1 Turbulent heating in high vertical wind shear

The first aspect to be discussed concerns the inherently strong vertical wind shear associated with turbulence, which makes the effect of turbulent heating on PV different from other diabatic processes that can occur in regions with modest vertical wind shear, such as latent heating in clouds or radiative heating. For easier explanation, we focus on the heating terms (terms 1 and 3) of Eq. (11) and rewrite their sum as:

$$\begin{aligned} & \frac{1}{\rho} \left[-\frac{\partial}{\partial y} \underbrace{\left(-\dot{\theta} \frac{\partial m}{\partial z} \right)}_1 - \frac{\partial}{\partial z} \underbrace{\left(\dot{\theta} \frac{\partial m}{\partial y} \right)}_3 \right] \\ &= \frac{1}{\rho} \left(\underbrace{\frac{\partial \dot{\theta}}{\partial y} \frac{\partial m}{\partial z}}_{\text{horizontal}} - \underbrace{\frac{\partial \dot{\theta}}{\partial z} \frac{\partial m}{\partial y}}_{\text{vertical}} \right). \end{aligned} \quad (14)$$

At synoptic scales, the horizontal length scale L is typically two orders of magnitude larger than the vertical scale H (i.e., $L/H \sim 10^2$). If there is a general diabatic heating source $\dot{\theta}$, its variations in the vertical direction are then larger than the ones in the horizontal direction by two orders of magnitude (i.e., $\frac{\partial \dot{\theta}}{\partial z} / \frac{\partial \dot{\theta}}{\partial y} \sim \frac{L}{H} \sim 10^2$). Therefore, the vertical term of Eq. (14) is dominant in modifying PV if the ambient vertical wind shear is weak and the heating source will generate the typical vertical dipole of PV tendencies, with positive tendency below and negative tendency above the heating maximum (assuming positive absolute vorticity; e.g., Wernli and Davies, 1997). However, if the vertical wind shear $\frac{\partial m}{\partial z}$ is large and roughly two orders of magnitude greater than the vertical component of absolute vorticity ζ_a (i.e., $\frac{\partial m}{\partial y}$), the horizontal term will be comparable to the vertical term and contribute significantly to PV modification (Chagnon and Gray, 2009).

In mid-latitudes, $\frac{\partial m}{\partial y}$ scales typically to 10^{-4} s^{-1} . Typical regions where we expect significant vertical wind shear and turbulence are above and below the upper-level jet core. A conservative approximation of the vertical wind shear can be made by assuming a jet with a maximum speed of 50 m s^{-1} and spanning a height of 5 km. The vertical wind shear then scales to 10^{-2} s^{-1} , which possesses the order of magnitude required to make the horizontal term important. Consequently, the horizontal term in Eq. (14) always has to be accounted for in the case of turbulent heating in jet environments and creates a horizontal dipole superimposed on the vertical one.

It should be noted that these arguments are also valid in the three-dimensional flow and the effect of diabatic heating in the presence of vertical wind shear has already been explored previously, for instance, in the context of embedded convection in warm conveyor belts (e.g., Harvey et al., 2020; Oertel et al., 2020). While these studies arrive at a similar conclusion as the one presented here, in the case of convection it is argued that the horizontal term becomes important because the heating source has a sub-synoptic-scale in the horizontal (L being smaller). This argument is not necessary for turbulent heating as the vertical wind shear is intrinsically high. Therefore, this specific characteristic of turbulence distinguishes it from other diabatic processes like latent heating or radiative heating when the effect on PV modification is concerned.

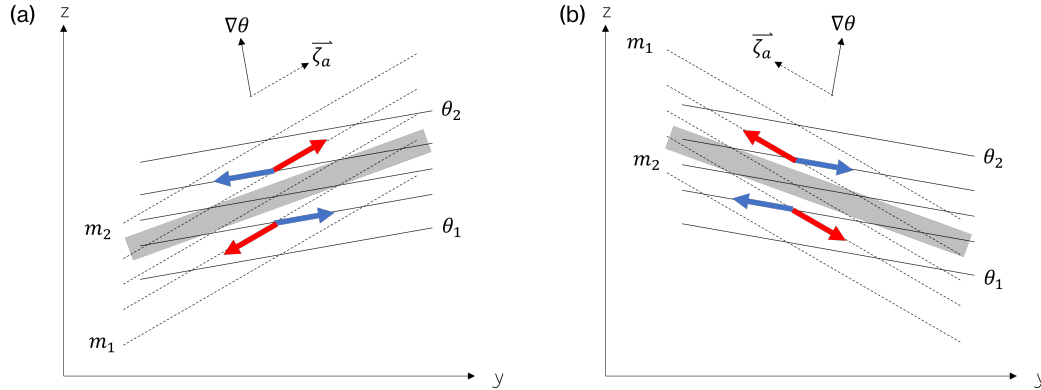


Figure 3. Illustration of the counteracting effect of $\mathbf{H}$ (directions indicated by the red arrows) and $\mathbf{M}$ (directions indicated by the blue arrows) in the yz plane for statically stable configurations with (a) $\frac{\partial m}{\partial z} > 0$ and (b) $\frac{\partial m}{\partial z} < 0$. The turbulent layer (grey shading) is tilted and assumed to be aligned with isotachs. The isentropes (solid lines) and isopleths of m (dashed lines) are plotted with $\theta_2 > \theta_1$ and $m_2 > m_1$. The directions of $\nabla\theta$ and ζ_a are indicated at the top. $\frac{\partial\theta}{\partial y}$ and $\frac{\partial m}{\partial z}$ are of opposite signs, consistent with thermal wind balance. The angles between $\mathbf{H}$ and $\mathbf{M}$ are always larger than 90° , which depicts the counteracting effect.

4.2 Counteracting effect of turbulent heat and momentum transfer

Another characteristic of the PV modification due to turbulence in this idealised framework is the counteracting effects of turbulent heat and momentum transfer in modifying PV. As discussed in Sect. 3.2, the vectors $\mathbf{H}$ and $\mathbf{M}$ represent the non-advective PV fluxes due to heat and momentum transfer, respectively. It is found that the $\mathbf{H}$ and $\mathbf{M}$ vectors usually point away from each other and counteract each other's transfer of PV. This follows directly from the mathematical form of these vectors (Eq. 12) and the usual acute angle between isentropes and isopleths of m .

To show this, the counteracting effect can be defined mathematically by computing the scalar product of $\mathbf{H}$ and $\mathbf{M}$. If the scalar product is negative, the angle between the two vectors is greater than 90° and we say that $\mathbf{H}$ and $\mathbf{M}$ are counteracting each other's effect on the PV modification. For the scalar product, we get:

$$\mathbf{H} \cdot \mathbf{M} = -\dot{\theta}\dot{u} \left(\frac{\partial m}{\partial z} \frac{\partial \theta}{\partial z} + \frac{\partial m}{\partial y} \frac{\partial \theta}{\partial y} \right). \quad (15)$$

We first limit our discussion to statically ($\frac{\partial\theta}{\partial z} > 0$) and inertially stable ($f \frac{\partial m}{\partial y} < 0$, e.g., Holton and Hakim, 2013) cases, as unstable cases are comparatively short-lived. Assuming $f > 0$, inertial stability infers $\frac{\partial m}{\partial y} < 0$. Then we can examine the two cases where $\frac{\partial m}{\partial z} = \frac{\partial u}{\partial z}$ is positive and negative, respectively. When $\frac{\partial m}{\partial z} > 0$, $\dot{\theta}\dot{u} > 0$ (Fig. 2a). If $\frac{\partial\theta}{\partial y} < 0$, the scalar product is negative. This is the case if $\frac{\partial\theta}{\partial y} \propto -f \frac{\partial u}{\partial z}$ ($f > 0$), as expected from thermal wind balance. When $\frac{\partial m}{\partial z} < 0$, $\dot{\theta}\dot{u} < 0$ (Fig. 2b) and the scalar product is negative if $\frac{\partial\theta}{\partial y} > 0$. Therefore, in a region that is statically and inertially stable, the scalar product $\mathbf{H} \cdot \mathbf{M}$ is always negative if the sign of the horizontal potential temperature gradient $\frac{\partial\theta}{\partial y}$ is in accordance with thermal wind balance. The heat and momentum transfer thus counteract each other when these conditions are fulfilled. The same conclusion can be obtained if one starts by assuming a statically and symmetrically stable situation (i.e., $\frac{\partial\theta}{\partial z} > 0$ and $Q > 0$).



Normally, this “thermal-wind-consistent” condition is fulfilled in the mid-latitude UTLS. Also, to obtain a positive scalar product $\mathbf{H} \cdot \mathbf{M}$, it is necessary to have $\left| \frac{\partial m}{\partial y} \frac{\partial \theta}{\partial y} \right| > \left| \frac{\partial m}{\partial z} \frac{\partial \theta}{\partial z} \right|$. However, as horizontal variations are typically orders of magnitude smaller than vertical variations, it is difficult to fulfil this condition. Consequently, the counteracting effect of turbulent heat and momentum transfer should be observed in almost all mid-latitude atmospheric flow in the UTLS.

These considerations can be illustrated using the two cases depicted in Fig. 3. The grey shading indicates the turbulent layer similar to the one discussed in Fig. 2. Both cases are statically, inertially and symmetrically stable. Figure 3a shows the case with $\frac{\partial u}{\partial z} > 0$ and we expect $\dot{u}$ and $\dot{\theta}$ to be negative above and positive below this layer. Potential temperature θ is decreasing in the y -direction, as expected from thermal wind balance. Similarly, Fig. 3b shows the case with $\frac{\partial u}{\partial z} < 0$ and $\frac{\partial \theta}{\partial y} > 0$, which is consistent with thermal wind balance. The directions of $\mathbf{H}$ and $\mathbf{M}$ vectors are then worked out and indicated by the red and blue arrows, respectively. The figure shows that the angle between $\mathbf{H}$ and $\mathbf{M}$ is always greater than 90° , leading to the counteracting effect of the heat and momentum transfer as discussed before.

4.3 Divergent flux from the turbulent layer

The last characteristic concerns the combined effect of heat and momentum transfer by turbulence $\mathbf{H} + \mathbf{M}$ on PV modification. We focus on the turbulent layer and therefore the region of strong wind shear, and consider the flux distribution relative to the closely spaced isotachs. However, we first discuss the flux distribution relative to isentropes and isopleths of m due to their simpler mathematical form. The total non-advective PV flux due to turbulence is:

$$\mathbf{H} + \mathbf{M} = \left(-\dot{\theta} \frac{\partial m}{\partial z} + \dot{u} \frac{\partial \theta}{\partial z}, \dot{\theta} \frac{\partial m}{\partial y} - \dot{u} \frac{\partial \theta}{\partial y} \right), \quad (16)$$

and we examine its effect on the turbulent layer and its surroundings by computing its scalar product with $\nabla \theta$, ∇m and ∇u , which indicates how PV is transferred by turbulence with respect to the instantaneous distribution of isentropes, isopleths of m , and isotachs. A positive value of the scalar product implies an up-gradient flux while a negative value implies a down-gradient flux.

Starting with θ and m , we obtain:

$$(\mathbf{H} + \mathbf{M}) \cdot \nabla \theta = \mathbf{H} \cdot \nabla \theta = -\dot{\theta} \left(\frac{\partial \theta}{\partial y} \frac{\partial m}{\partial z} - \frac{\partial \theta}{\partial z} \frac{\partial m}{\partial y} \right) \quad (17a)$$

$$(\mathbf{H} + \mathbf{M}) \cdot \nabla m = \mathbf{M} \cdot \nabla m = -\dot{u} \left(\frac{\partial \theta}{\partial y} \frac{\partial m}{\partial z} - \frac{\partial \theta}{\partial z} \frac{\partial m}{\partial y} \right). \quad (17b)$$

The scalar product with $\nabla \theta$ only depends on $\dot{\theta}$ as $\mathbf{M}$ is parallel to isentropes while that with ∇m only depends on $\dot{u}$ as $\mathbf{H}$ is parallel to isopleths of m . The two products share the same term in brackets, which relates to Q as shown in Eq. (12a). Therefore, if $Q > 0$ in the region considered, the term in brackets is positive and the scalar products have the opposite sign of $\dot{\theta}$ and $\dot{u}$, respectively.

We again focus on statically stable conditions and first consider the situation where $\frac{\partial m}{\partial z} > 0$ (Fig. 3a). The scalar product is then positive above the layer and negative below the layer. It implies that the up-gradient flux above the layer is pointing upward and the down-gradient flux below the layer is pointing downward. Therefore, the total non-advective PV flux due to



turbulence diverges from both the isentropes and isopleths of m near the turbulent layer, transferring PV away. For the situation where $\frac{\partial m}{\partial z} < 0$ (Fig. 3b), as the sign of $\dot{u}$ is reversed across the turbulent layer, the scalar product is negative above the layer and positive below the layer. However, as $\frac{\partial m}{\partial z} < 0$, the up- and down-gradient directions are reversed as well. As a result, the flux again diverges in this configuration. This result is also obvious from Fig. 3, with $\mathbf{H}$ diverging from isentropes and $\mathbf{M}$ diverging from isopleths of m near the turbulent layer.

It is important to note that the non-advective PV flux actually does not cross isentropic surfaces and the statement “PV is being transferred away from isentropes” here refers only to the instantaneous distribution of isentropes. When the movement of isentropic surfaces is accounted for, the impermeability theorem for PV remains satisfied (Haynes and McIntyre, 1987). Also, while Fig. 3 only displays the configurations that satisfy the “thermal-wind-consistent” condition, this condition is not required in the above derivation and hence, the total non-advective PV flux due to turbulence is always divergent from isentropes and isopleths of m provided that PV is positive in the statically stable region.

The transfer of PV with respect to isotachs is more involved as neither $\mathbf{H}$ nor $\mathbf{M}$ are parallel to the isotachs. The scalar product:

$$(\mathbf{H} + \mathbf{M}) \cdot \nabla u = -\dot{u} \left(\frac{\partial \theta}{\partial y} \frac{\partial u}{\partial z} - \frac{\partial \theta}{\partial z} \frac{\partial u}{\partial y} \right) - \dot{\theta} f \frac{\partial u}{\partial z}, \quad (18)$$

therefore, depends on both heat and momentum transfer terms. However, careful analysis (see Appendix B1 for details) shows that the total non-advective PV flux due to turbulence is diverging from the isotachs near the turbulent layer in most situations if the region of interest is statically stable and has positive PV. For the opposite to occur (i.e., the flux converges towards isotachs), two strict conditions must be satisfied at the same time:

$$\begin{cases} \frac{\partial u}{\partial y} / \frac{\partial u}{\partial z} > \frac{\partial \theta}{\partial y} / \frac{\partial \theta}{\partial z} > (\frac{\partial u}{\partial y} - f) / \frac{\partial u}{\partial z} & \text{if } \frac{\partial u}{\partial z} > 0 \\ \frac{\partial u}{\partial y} / \frac{\partial u}{\partial z} < \frac{\partial \theta}{\partial y} / \frac{\partial \theta}{\partial z} < (\frac{\partial u}{\partial y} - f) / \frac{\partial u}{\partial z} & \text{if } \frac{\partial u}{\partial z} < 0, \end{cases} \quad (19)$$

and

$$\left| \dot{u} \left(\frac{\partial \theta}{\partial y} \frac{\partial u}{\partial z} - \frac{\partial \theta}{\partial z} \frac{\partial u}{\partial y} \right) \right| > \left| \dot{\theta} f \frac{\partial u}{\partial z} \right|. \quad (20)$$

Specifically, Eq. (19) requires precisely the isentropes to slope steeper than the isotachs, but less steep than the isopleths of m . This condition is even more restrictive when the vertical wind shear is strong (see Appendix B1 for details), causing a convergent non-advective PV flux towards the turbulent layer highly unlikely. Equation (20) states that the scalar product for the momentum transfer term $\mathbf{M} \cdot \nabla u$ must also be larger in magnitude compared to that for the heat transfer term $\mathbf{H} \cdot \nabla u$ simultaneously. Consequently, the total non-advective PV flux due to turbulence should be divergent from the isotachs as well near the turbulent layer in most situations, given that $\frac{\partial \theta}{\partial z} > 0$ and $Q > 0$.

4.4 Summary

Based on flux-gradient theory to describe the effect of turbulence and adopting the quasi-two-dimensional approximation, three characteristics of the effect of turbulence on PV modification have been derived thus far:



- The high vertical wind shear inherently associated with the occurrence of turbulence makes the horizontal terms in the scalar product in the equation of diabatic PV modification (i.e., the horizontal non-advective PV fluxes) important. This is different from other diabatic heating processes, which may occur in an environment with low vertical wind shear.
 - Turbulent heat and momentum transfer have a counteracting effect on PV modification, provided that the configuration is statically stable, inertially or symmetrically stable, and “thermal-wind-consistent”. The non-advective PV fluxes due to the heat H and momentum M transfer terms are pointing away from each other (i.e., their scalar product is negative). This counteracting effect is then also manifested in the PV modification (Eq. 11).
 - The total non-advective PV flux due to turbulence, $H + M$, is divergent from the turbulent layer (assumed to be the layer with the strongest wind shear) in most cases if the configuration is statically and symmetrically stable. A non-advective PV flux convergence towards the turbulent layer is possible only if conditions stated in Eq. (19) and (20) are both satisfied, which is seldom realised in reality (see Appendix B1 for details). Therefore, PV is usually transferred away from the turbulent layer by the divergent fluxes.
- Nonetheless, the idealised framework with a single turbulent layer discussed in this section may oversimplify the complex atmospheric flow in reality. It is therefore important to verify whether these characteristics can be observed in realistic atmospheric flows as simulated with state-of-the-art NWP models that use the flux-gradient approach to parametrise turbulence.

5 Representation of PV modification by turbulence in the IFS simulation

To check whether the simplified framework applies to realistic atmospheric flows, we consider a vertical section normal to an intense upper-level jet over the North Atlantic with peak winds exceeding 75 m s^{-1} simulated by the IFS (Fig. 4). Such a cross section most likely satisfies the quasi-two-dimensional approximation used in the previous section (with the jet axis serving as the coherent direction). The PV and PV tendencies shown in Fig. 4 are first calculated in their three-dimensional form and interpolated to the cross section. As shown in Fig. 4a, there is a prominent tropopause fold that extends to below 500 hPa and coincides with closely spaced isentropes. The whole system is then referred to as the upper-level jet-front system, and qualitatively resembles the flow situations investigated in previous studies (e.g., Shapiro, 1976; Spreitzer et al., 2019). From this vertical section, we first examine if the assumptions in Sect. 4 are realised. A prominent assumption was that PV is positive in the region of interest, which is satisfied in most regions of the cross section, except for some localised regions on the anticyclonic side of the jet core. The atmosphere is also statically ($\frac{\partial \theta}{\partial z} > 0$) and inertially stable ($f \frac{\partial m}{\partial y} < 0$), and the “thermal-wind-consistent” condition (i.e., $\frac{\partial \theta}{\partial y} \propto -f \frac{\partial u}{\partial z}$) is also fulfilled in general in this upper-level jet-front system. As these conditions are generally satisfied, we proceed to examine the effects of turbulence on PV modification in this flow situation.

Figures 4b, c show the instantaneous tendencies of potential temperature $\dot{\theta}$ and momentum $\dot{u}$ (normal to the cross section) due to the turbulence parametrisation in the model and they are used to calculate the PV tendencies. The $\dot{\theta}$ and $\dot{u}$ fields display clear dipole structures in the frontal zones above and below the jet core, assuring that the idealised vertical profiles in Fig. 2 are consistent with the turbulent fluxes simulated by the IFS in a classical upper-level jet-front system. The dipoles are also

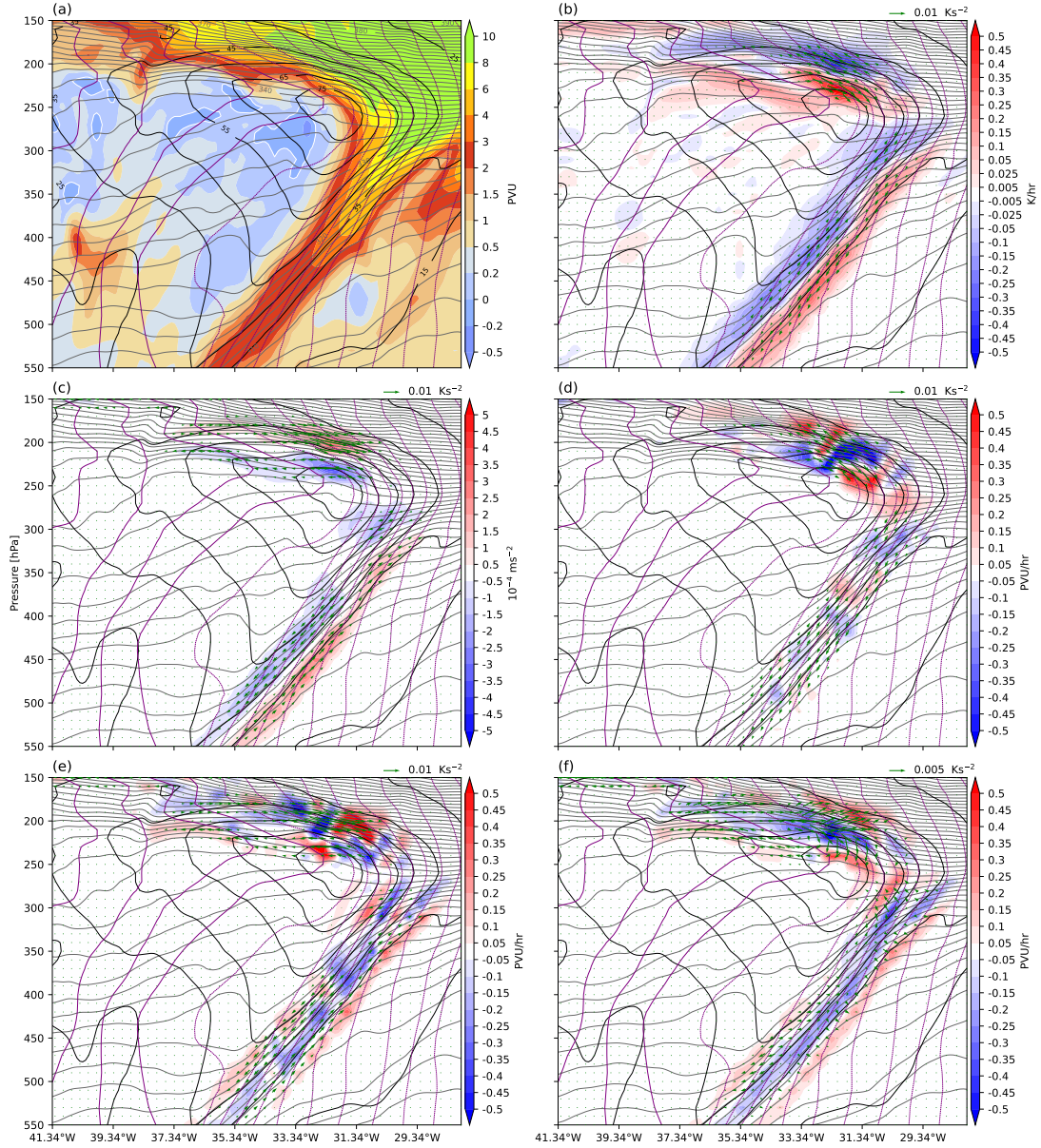


Figure 4. Vertical section across an upper-level jet at 12 UTC on 30 August 2019 showing (a) PV, (b) $\dot{\theta}$, (c) $\dot{u}$, (d) PV tendency due to turbulent heat transfer, (e) PV tendency due to turbulent momentum transfer, and (f) PV tendency due to turbulence. Isentropes (grey contours, 2 K interval), isotachs of wind normal to the cross section (black contours, 10 m s^{-1} interval), and isopleths of absolute momentum m (purple contours, 10 m s^{-1} interval) are overlaid. The green arrows indicate the vector fields (b,d) $-\zeta_a \dot{\theta}$, (c,e) $\nabla \theta \times \mathbf{F}$, and (f) $-\zeta_a \dot{\theta} + \nabla \theta \times \mathbf{F}$ projected onto the cross section, and they are approximately equal to (b,d) $\mathbf{H}$, (c,e) $\mathbf{M}$, and (f) $\mathbf{H} + \mathbf{M}$. Note that the arrows in (f) are enlarged by a factor of 2 compared to (b-e).



435 located in regions with enhanced vertical wind shear, in agreement with our expectation. The green vectors overlaid in Fig. 4b, c are the projections of the vector fields $-\zeta_a \dot{\theta}$ and $\nabla \theta \times \mathbf{F}$, respectively, onto the cross section. If the quasi-two-dimensional approximation is valid, terms related to the variations in the x -direction are negligible (see Eq. A1) and the projections reduce to $\mathbf{H}$ and $\mathbf{M}$. This is demonstrated by the alignment of green arrows in Fig. 4b with the isopleths of m , following Eq. (12c), and that in Fig. 4c with the isentropes, consistent with Eq. (12d).

440 Several properties of the turbulence-induced non-advective PV flux discussed in Sect. 3 and 4 can also be observed in this cross section (Fig. 4b, c). First, the projected vectors generally have a significant horizontal component (especially those associated with the dipole above the jet core), recalling the discussion in Sect. 4.1 on the role of vertical wind shear in PV modification due to turbulence. Moreover, when comparing the two sets of vectors, the counteracting effect of heat and momentum transfer by turbulence on the PV modification discussed in Sect. 4.2 is evident. Taking the dipole above the jet core as an example, 445 the heat transfer induces a flux predominantly towards the left in the cooling region while the momentum transfer induces a flux predominantly towards the right in the corresponding location. The same occurs in the heating region, but with the fluxes pointing to the right for the heat transfer term and to the left for the momentum transfer term. This counteracting effect is also evident across the dipole pattern in the frontal zone below the jet, even though the vectors have a smaller magnitude.

The PV tendencies due to turbulent heat and momentum transfer are separately shown in Fig. 4d, e, together with the 450 corresponding projection of $-\zeta_a \dot{\theta}$ and $\nabla \theta \times \mathbf{F}$. The prominent positive and negative PV tendencies are generally found in regions with notable convergence and divergence of the projected non-advective PV fluxes, suggesting that the fluxes normal to the cross section have minimal contribution. As the fluxes possess significant horizontal components, the pattern of PV tendencies due to heating deviates from the typical vertical pattern. From Fig. 4b, one may expect a vertically-oriented positive-negative-positive PV tendency tripole pattern due to the turbulent heat transfer above the jet core, with the negative region in 455 the centre of the heating and cooling dipole. However, as Fig. 4d displays, the PV tendency due to turbulent heat transfer has a different pattern, forming along the direction where the fluxes converge or diverge most significantly. It once more emphasises the important role of vertical wind shear (Sect. 4.1). The PV tendencies induced by turbulent momentum transfer form an interesting quadrupole above the jet core (Fig. 4e) due to the isolated dipole of momentum tendencies at the same location (Fig. 4c). The quadruple pattern occurs because the isentropes and the isotachs (parallel to the turbulent layer) have very 460 similar slopes, with the former restricting the flux $\nabla \theta \times \mathbf{F}$ to align with the momentum tendency dipole.

Figure 4f shows the total PV tendency due to turbulence and the vector field $-\zeta_a \dot{\theta} + \nabla \theta \times \mathbf{F}$ projected onto the cross section (i.e., the sum of Fig. 4d, e). The vectors are enlarged for better visualisation since the counteracting effect between turbulent heat and momentum transfer reduces their magnitudes. The resultant vector field again shows that its convergence and divergence can be used to infer PV tendencies. The total PV tendencies due to turbulence form a vertical tripole pattern 465 above the jet and a similar but tilted tripole pattern in the tropopause fold region. In both regions, PV is transferred away from the turbulent layer (inferred from the dipoles in Fig. 4b, c), which is consistent with the discussion in Sect. 4.3. The divergent fluxes leave their signatures as coherent PV tendency tripole patterns due to turbulence. These tripole patterns are striking, as they are very clear in Fig. 4f, but neither observable in Fig. 4d nor e. Therefore, these instantaneous tripole patterns are the result of the complex interplay between turbulent heat and momentum transfer, highlighting that contributions from both



the heat and the momentum fluxes are essential in this case. We can also connect this tripole pattern to the elongated bands observed in Fig. 1, by assuming this tripole extends horizontally along the jet axis. The idealised framework thus provides a mechanistic explanation for the emergence of these banded structures.

Similar tripolar signals were also identified by Spreitzer et al. (2019) in their composite cross section, although they attributed their formation mainly to the effect of turbulent heat fluxes, as suggested by Shapiro (1976). Nevertheless, the cross sections here (Fig. 4d-f) demonstrate that the tripolar patterns can emerge as a result of both turbulent heat and momentum fluxes. If we focus on the tripole below the jet core, the contribution from momentum fluxes appears to dominate. The relative contribution from heat and momentum transfer is likely dependent on the background gradients and the relative alignment of isentropes and isotachs (see Fig. 3), which vary across different situations. The below-jet tripole also coincides with the tropopause fold (Fig. 4a) and it is effectively “mixing” the high PV within the fold to its surroundings. Similar tripoles of PV tendency were also found in a numerical simulation of the decay of a tropopause fold using a two-dimensional isentropic model with turbulence parametrised (Hartjenstein, 2000).

To summarise, the properties and characteristics of PV modification due to turbulence discussed in Sect. 3 and 4 can mostly be observed in the vertical cross section shown in Fig. 4, which is valid for a jet-front system as simulated by the IFS. The applicability of the idealised quasi-two-dimensional framework to realistic atmospheric flows is justified by the consistency between the characteristics derived and those observed in the simulation. This framework is therefore useful in understanding how turbulence modifies PV in the UTLS region. An important result we learned is that the divergent non-advective PV flux from the turbulent layer in quasi-two-dimensional jet-front systems generates coherent tripole patterns in the instantaneous PV tendency field both above and below the jet. This tripolar signal was also found in previous studies (e.g., Hartjenstein, 2000; Spreitzer et al., 2019) and we now provide a mechanistic explanation for its formation.

6 Accumulated PV changes due to turbulence

The previous sections showed that turbulence can induce a structured PV tendency tripole instantaneously, which extends horizontally along the coherent direction and forms elongated PV tendency bands. This spatial coherence provides the essential first step for the effect of turbulence on PV modification to be significant for the large-scale flow. Spreitzer et al. (2019) found that the above-jet trippole is present in both the instantaneous PV tendency and in the accumulated PV changes (their Fig. 7c and 4c), indicating that significant material PV changes can be induced by turbulence. However, if an air parcel is advected through regions with PV tendencies of alternating signs, the individual PV changes may be neutralised when accumulated over time. Therefore, for the effect of turbulence to be important, we have to examine whether prominent PV changes due to turbulence do accumulate along the flow.

6.1 Importance of the accumulated effect of turbulence

As outlined in Sect. 2.3, we integrate the PV tendencies for different parametrisation schemes along backward trajectories using the reverse domain filling method. Figures 5a, b display the material PV change (ΔQ) and the total APV in the previous 12 h

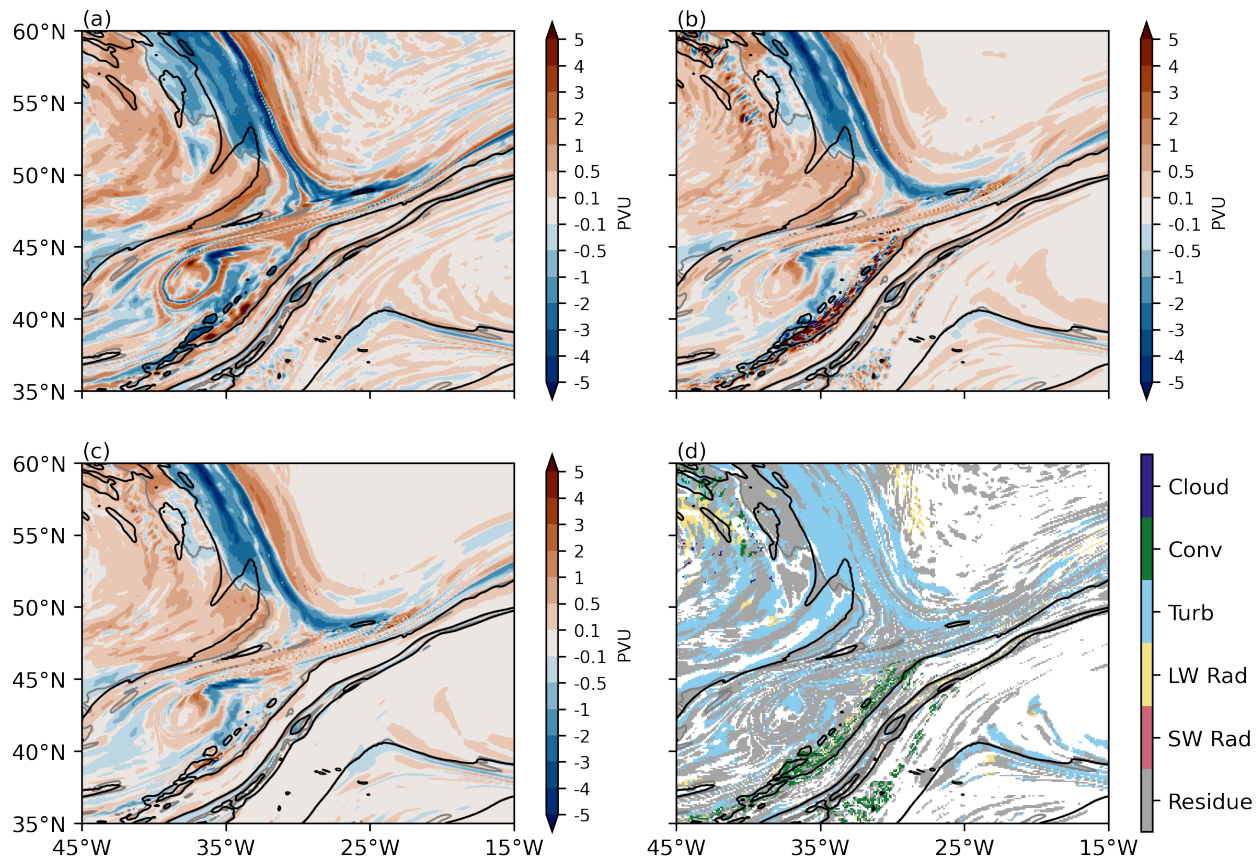


Figure 5. Results from the analysis of Lagrangian PV modification: (a) ΔQ , (b) total APV, (c) APV due to turbulence, and (d) the dominant processes attributed to ΔQ with an accumulation time of 12 h on 200 hPa at 12 UTC on 30 August 2019. The black and grey lines indicate the 2-PVU contours of PV and the advected PV from 12 h ago, respectively. Grid points with $|\Delta Q| < 0.2$ PVU are masked in (d). Labels for processes: Cloud: cloud microphysics; Conv: convection; Turb: turbulence; LW Rad: longwave radiation; SW Rad: shortwave radiation.

of trajectories initialised on 200 hPa at the same time as Fig. 4. The two fields are very similar, especially when considering the large-scale features. For instance, both fields indicate a broad region of PV decrease stretching along the western flank of the trough, with another elongated band of PV increase immediately to its east. Also, there is a hook-shaped region within the cutoff showing a decrease in PV in both fields. Some differences can still be found between the two fields, but they are mostly limited to fine-scale features, like the small filaments deep in the stratosphere within the trough and the cutoff. The general similarity between ΔQ and the total APV justifies the usage of the integration method to infer the underlying processes that modify PV. The sensitivity of the features in the total APV field to the accumulation time and the temporal evolution of these features are examined further in (Lee, 2025, their Chapter 6.3). The results indicate that the large-scale APV features develop



steadily and evolve coherently in time. Consequently, though the results presented here are based on a single accumulation time and at one time instant, they can be considered as representative.

We next examine the APV field of individual parametrised processes. APV due to turbulence only (Fig. 5c) contains most of the large-scale features of the total APV (Fig. 5b), especially in the region along the section of the upper-level jet-front system examined in Sect. 5. It illustrates that these elongated and coherent bands of positive and negative APV along the jet are likely generated by turbulence. To confirm this, we use the process attribution method outlined in Sect. 2.3 to assign each trajectory a process as the dominant cause of ΔQ , with the residue term taken into account (the cause is uncertain if the residue is dominating ΔQ). The result is shown in Fig. 5d and the APV bands discussed are indeed mainly caused by turbulence, amid some scattered regions with uncertain causes. Furthermore, turbulence is the main cause of the PV changes on this isobaric surface, with longwave radiation and convection dominating only in small regions in the upstream ridge and on the southeastern side of the cutoff.

From Fig. 5, we can also examine how the dynamical tropopause is modified by turbulence in the past 12 h. The black and grey lines show the 2-PVU contours of the current and 12-h advected PV fields, respectively. On the western flank of the trough near 50°N, there is a significant mismatch between the contours, with ΔQ mostly attributed to turbulence. This reveals that the shape of the dynamical tropopause was locally modified due to upstream turbulence in the previous 12 h.

The total APV and the results of the process attribution on 350 and 500 hPa are shown in Fig. 6. Total APV displays clear elongated bands along the western flank of the trough (Fig. 6a, c) that extend even to the downstream side. The dominant cause of ΔQ for these bands is again turbulence (Fig. 6b, d). In particular, the positive-negative-positive arrangement of the bands on 350 hPa recalls the tripolar signal of the instantaneous PV tendency due to turbulence below the jet core in the vertical section examined (Fig. 4f). This signal further extends along the tropopause fold (the large region surrounded by the black contour in Fig. 6c) down to 500 hPa with a slightly weakened magnitude.

Compared to 200 hPa, there are more regions with ΔQ attributed to processes other than turbulence at lower altitudes (Fig. 6b and d). For instance, longwave radiation dominates the PV increase within the cutoff on 350 hPa. Cloud processes and convection are responsible for the spotty ΔQ on the downstream flank of the cutoff and the trough, as well as the PV changes in the upstream ridge. Nevertheless, turbulence remains the dominant process for ΔQ near the upper-level jet-front system. Moreover, the PV changes induced by turbulence clearly modify the tropopause fold in the past 12 h, with some tropospheric air incorporated into the fold on the eastern edge and some stratospheric air expelled on the northwestern side (compare black and grey contours). Examination of the same field on 600 hPa (not shown) indicates that a large part of the lowermost tip of the fold is dissipated by turbulence in the previous 12 h, consistent with the findings of Hartjenstein (2000) and Spreitzer et al. (2019). These results not only demonstrate that turbulence may induce coherent material PV changes, but also indicate that the effect of turbulence on PV modification in the UTLS region is important quantitatively.

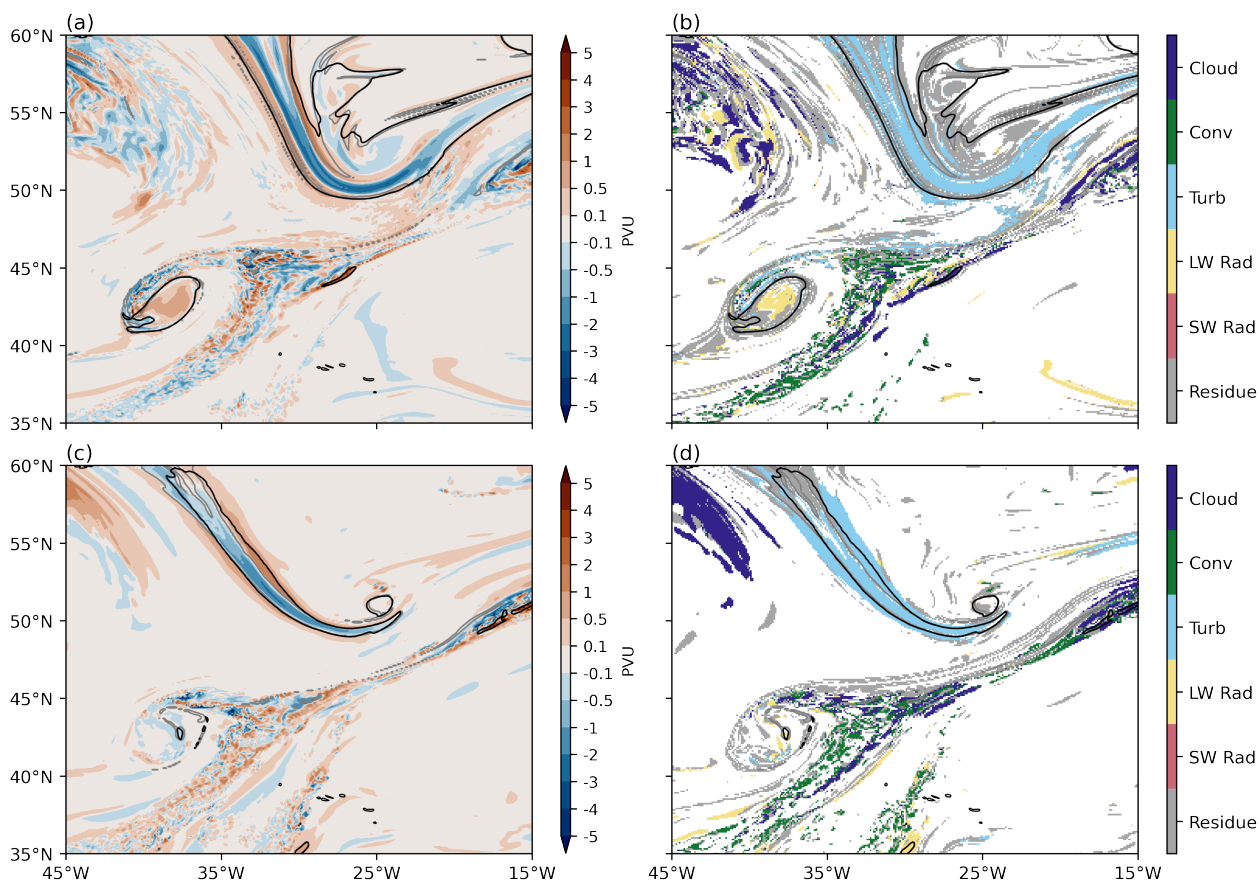


Figure 6. Similar to Fig. 5b, d, but (a, b) on 350 hPa and (c, d) on 500 hPa. (a, c) show total APV and (b, d) the dominant processes attributed to ΔQ with an accumulation time of 12 h.

6.2 Formation of coherent material PV changes

As illustrated above, the elongated APV bands identified on the western flank of the trough have a pattern similar to those identified for the instantaneous PV tendency due to turbulence in Fig. 1 and 4, indicating a close linkage. To understand how these elongated APV bands are built along the flow, we explore the Lagrangian history of selected air parcels within the bands.

First, we examine the elongated bands of APV on 200 hPa near the jet on the upstream flank of the trough, shown in Fig. 7a. Four selected 12-h backward trajectories are overlaid, all having turbulence attributed as the dominant process contributing to their 12-h ΔQ . The trajectories are initiated on 200 hPa from the locations indicated by the white circles. For easy reference, the trajectories and the air parcels they represent will be referred to by the label of the figure, which shows the temporal evolution of the vertical profile of PV tendency due to turbulence along the trajectory. For instance, the red trajectory in Fig. 7a, which is further portrayed in Fig. 7b, will be referenced as trajectory ‘7b’.

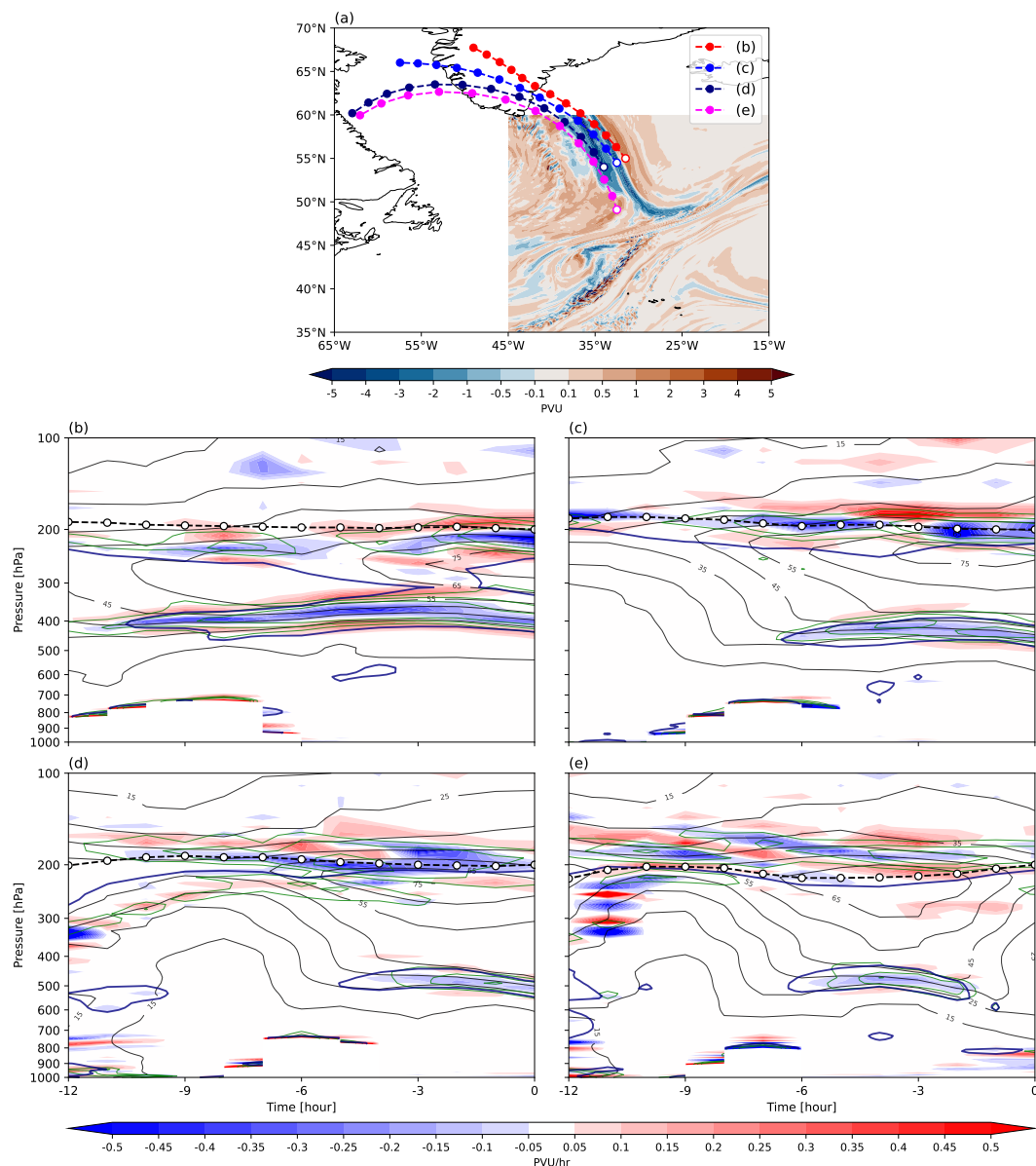


Figure 7. (a) Total APV on 200 hPa at 12 UTC on 30 August 2019 with an accumulation time of 12 h (same field as shown in Fig. 5b but in a larger domain). Four backward trajectories are shown, labelled (b) to (e), and their horizontal positions in the last 12 h are shown by filled circles (white filling at $t = 0$ h). (b-e) Temporal evolution of the vertical profile of PV tendency due to turbulence (in colours) along the backward trajectories (dashed lines) with the corresponding label defined in (a). Contours show wind speed (grey, m s^{-1}), vertical wind shear (green, 0.015 to 0.03 s^{-1} at 0.005 s^{-1} intervals), and PV (blue for 2 PVU).



From the horizontal positions of the four trajectories, the strong horizontal shear in the upper-level jet is discernible. The distance travelled is the shortest by the easternmost air parcel ('7b'), then increases with the starting position being further west ('7c' to ('7e')), indicating an increase in wind speed towards the jet core on the western flank of the trough. Therefore, air parcels nearby at a specific time could have originated from substantially different regions, which indicates a major difference between instantaneous PV tendencies and accumulated PV changes .

We first consider the pair of trajectories to the east, with trajectory '7b' initiated from the positive APV band and trajectory '7c' from the negative APV band, and Fig. 7b, c shows the vertical profiles of the PV tendency due to turbulence along these trajectories. Both trajectories remain close to 200 hPa in regions with strong vertical wind shear above the jet core, where vertical tripoles of PV tendency are generated by turbulence. Air parcel '7b' encounters positive PV tendency as early as $t = -9\text{h}$ and continuously experiences an increase in PV after $t = -6\text{h}$ by entering the uppermost part of the tripole pattern. Air parcel '7c' accumulates negative PV tendencies in the previous 12 h as it travels continuously near the centre of the vertical tripole with negative PV tendencies. Recalling the vertical cross section shown in Fig. 4f, the two air parcels are likely advected along the tilted vertical tripole of PV tendency due to turbulence above the jet core in the last 12 h, resulting in a positive APV band located east of a negative one.

Following this argument, one would expect another positive APV band to the west of the negative band because of air parcels advected through the lower part of the PV tendency tripole, roughly at the starting position of trajectory '7d'. However, this region has mostly negative APV, with the expected positive APV only found further south around the starting position of trajectory '7e'. When the vertical profiles of PV tendency due to turbulence along these trajectories are examined (Fig. 7d, e), the tripole pattern can still be recognised, but the bands vary vertically with time and no longer form continuous bands. For instance, air parcel '7d' appears to transit from one tripole it travels through from $t = -10\text{h}$ to $t = -4\text{h}$ to another one from $t = -3\text{h}$ onward, and air parcel '7e' also records vertical displacements of the tripole pattern. These changes can be the result of temporal changes of the upper-level jet itself or the air parcels moving to a different part of the jet, but both possibilities demonstrate the complexity when comparing instantaneous PV tendencies and accumulated PV change. Though trajectory '7d' follows a similar pathway as trajectory '7e' only slightly later (Fig. 7a), the PV tendencies they experienced are significantly different. While the positive APV signal expected from the lower part of the PV tendency tripole is retained by air parcel '7e', air parcel '7d' has an opposite, negative APV value owing to such variations. A more pronounced positive APV band is found instead on 250 hPa (not shown here, see Lee, 2025), with its origin more clearly associated with the lower part of the PV tendency tripole.

Therefore, the APV features near the jet on the western flank of the trough on 200 hPa are mainly caused by the vertical tripolar pattern of PV tendency due to turbulence above the jet core. Nevertheless, with the spatio-temporal variations of the PV tendency field and the shear experienced by the air parcels, the footprint of the instantaneous PV tendency is manifested in various ways in the APV fields, leading to the formation of elongated APV bands, with some being less well defined or deformed.

We continue to examine the elongated APV bands at lower altitudes, especially the positive-negative-positive tripolar pattern at 350 hPa (Fig. 8a). The selected trajectories are again launched from grid points where ΔQ is dominated by turbulence

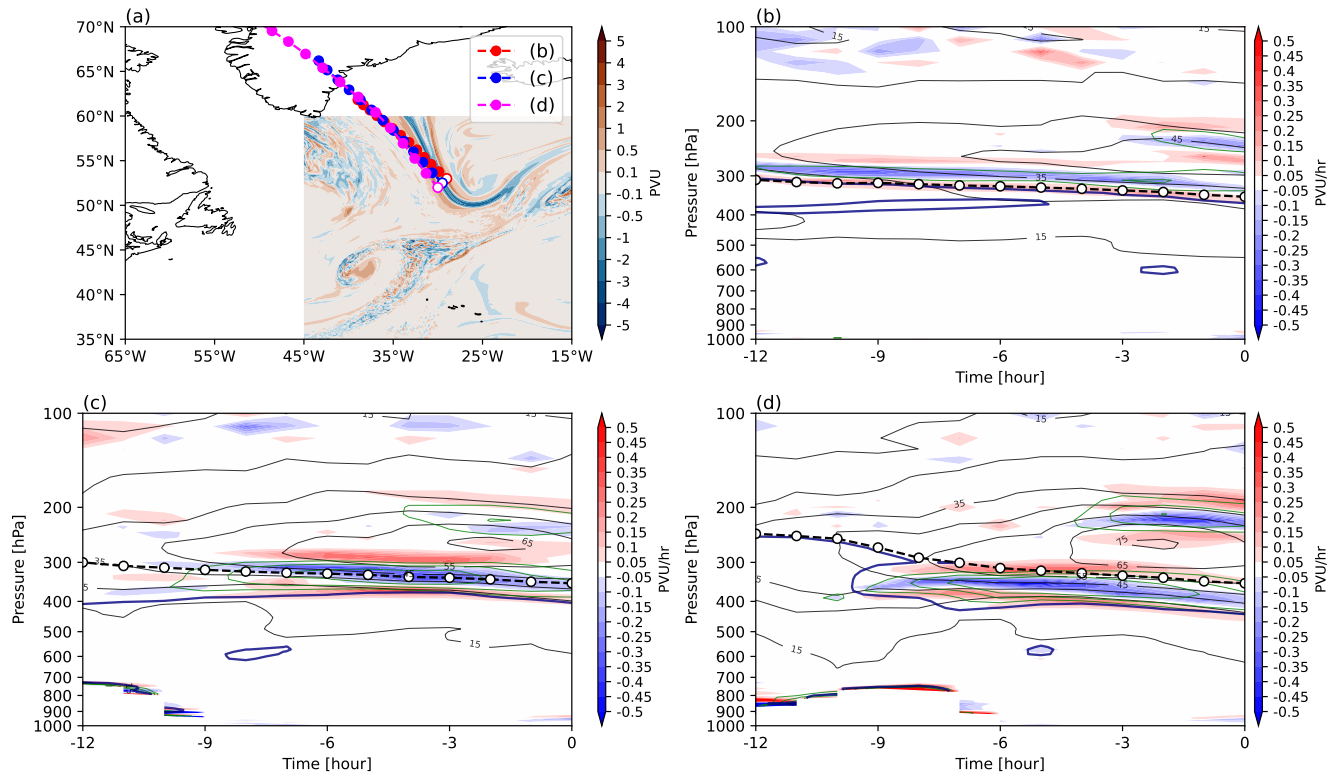


Figure 8. (a) Total APV on 350 hPa at 12 UTC on 30 August 2019 with an accumulation time of 12 h (same field as shown in Fig. 6a but in a larger domain). Three backward trajectories are shown, labelled (b) to (d), and their horizontal positions in the last 12 h are shown by filled circles (white filling at $t = 0$ h). (b-d) Temporal evolution of the vertical profile of PV tendency due to turbulence (in colours) along the backward trajectory (dashed lines) with the corresponding label defined in (a). Contours show wind speed (grey, m s^{-1}), vertical wind shear (green, 0.015 to 0.03 s^{-1} at 0.005 s^{-1} intervals), and PV (blue for 2 PVU).

contributions, and the vertical profiles of instantaneous PV tendency due to turbulence along these trajectories are shown in Fig. 8b-d. For all three trajectories, a clear tripolar pattern of instantaneous PV tendency due to turbulence appears in the sheared layer below the jet core at the levels where the trajectories pass through. Air parcel ‘8b’, with the easternmost starting position that is furthest from the jet core, moves comparatively more slowly and stays for the entire 12 h period in the lower part of the tripole with positive PV tendencies (Fig. 8b). In comparison, air parcel ‘8c’ is closer to the jet core, moves at a higher speed, enters the middle part of the tripole only around $t = -8$ h, and accumulates negative PV changes (Fig. 8c). Air parcel ‘8d’, which travels at the highest speed among the three, descends from around 250 hPa at $t = -12$ h to around 300 hPa at $t = -7$ h to enter the region of positive PV tendencies in the upper part of the tripole (Fig. 8d). These differences in the speed and the relative positions to the tripole pattern are all consistent with the vertical cross section shown in Fig. 4f, where a tilted tripole below the jet core emerges at around 300 hPa and stretches down into the tropopause fold (cf. Fig. 4a). Therefore, the

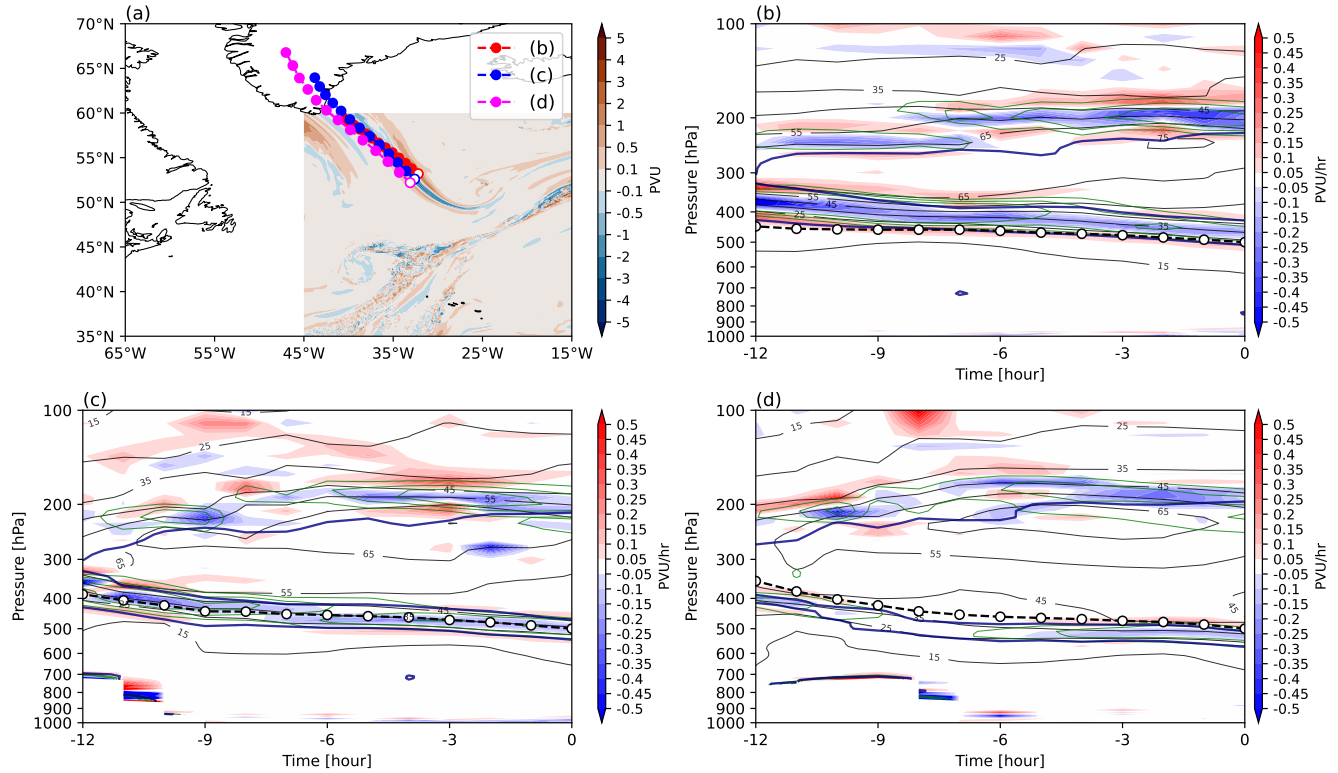


Figure 9. (a) Total APV on 500 hPa at 12 UTC on 30 August 2019 with an accumulation time of 12 h (same field as shown in Fig. 6c but in a larger domain). Three backward trajectories are shown, labelled (b) to (d), and their horizontal positions in the last 12 h are shown by filled circles (white filling at $t = 0$ h). (b-d) Temporal evolution of the vertical profile of PV tendency due to turbulence (in colours) along the backward trajectory (dashed lines) with the corresponding label defined in (a). Contours show wind speed (grey, m s^{-1}), vertical wind shear (green, 0.015 to 0.03 s^{-1} at 0.005 s^{-1} intervals), and PV (blue for 2 PVU).

elongated bands of APV are the manifestation of the time-integrated signals of PV changes of air parcels that steadily pass through the instantaneous tripole of PV tendency due to turbulence.

The same connection is also observable deep into the tropopause fold on 500 hPa, again due to coherent flows in tripolar bands of APV (Fig. 9a). The temporal evolutions of the vertical profiles of the three trajectories initiated from the easternmost positive (Fig. 9b), middle negative Fig. 9c), and westernmost positive APV bands (Fig. 9d), respectively, are analogous to the corresponding ones on 350 hPa, with the tripole sometimes being more intermittent. The accumulation of positive or negative PV tendency within the tripole explains the formation of the corresponding APV bands to which each trajectory belongs. Consequently, the APV bands at the tropopause fold can be primarily explained by the PV tendency tripole due to turbulence discussed previously in Sect. 5.

Summarising this Lagrangian analysis based on selected trajectories, we conclude that the elongated APV bands in proximity to the upper-level jet-front system are mostly formed by the steady accumulation of instantaneous PV tendencies due



to turbulence by individual air parcels. In the presence of strong shear, these APV bands at a given time are composed of air parcels originating from different locations and moving with vastly different speeds. In spite of this dynamical nature, the synoptic flow associated with the upper-level jet guides air parcels to consistently travel through a specific location relative to the PV tendency tripole pattern. The instantaneous PV changes induced by turbulence are therefore accumulated in time and the resultant elongated APV bands are almost an imprint of the instantaneous PV tendency pattern, which however extend further downstream due to advection. Turbulence may hence prominently and coherently modify PV, which via PV inversion, acts as a feedback of small-scale turbulence to the larger-scale, as illustrated in this upper-level jet-front system.

7 Discussion

7.1 Turbulence-induced pattern: Tripole or dipole?

A major result shown in the previous sections is the vertical tripolar pattern of PV tendency induced by turbulence in the upper-level jet-front system (Sect. 5), the existence of which can be understood with the help of the quasi-two-dimensional framework (Sect. 3 and 4). Furthermore, this tripolar pattern is manifested as elongated PV tendency bands on isobaric surfaces along the jet axis, and it is approximately preserved in the APV field (Sect. 6). Similar tripolar patterns were observed in previous studies (e.g., Hartjenstein, 2000; Spreitzer et al., 2019; Spreitzer, 2020), however, there is also an apparent contradiction with the results of Saffin et al. (2017), who found a pronounced vertical dipole pattern across the tropopause due to turbulent mixing in the composite of forecasts performed with the Met Office Unified Model using the PV tracers method (their Fig. 2 and 7).

We have no clear answer to resolve this discrepancy, but we would like to mention the caveats when comparing the two studies. First, the study presented here has quite a different methodology from that employed in Saffin et al. (2017), which makes a direct comparison not straightforward. For instance, our analysis is based on a case study, while Saffin et al. (2017) computed mean vertical profiles of numerous grid points from 92 forecasts. Also, the accumulation time in this study is chosen to be 12 h, which is shorter than the 24 h used by Saffin et al. (2017). More importantly, the dipole revealed in Saffin et al. (2017) is tropopause-relative, while the tripole discussed here is relative to the turbulent layer.

In an analysis presented in (Spreitzer, 2020, their Chapter 4), which is based on the same model as used here (an older version of the IFS) and the same Lagrangian PV diagnostics method, but with other aspects of the methodology almost equivalent to those of Saffin et al. (2017), a tripolar pattern across the tropopause was found in ridge regions. As Spreitzer (2020) pointed out, this discrepancy to Saffin et al. (2017) could also be the result of the differences in the numerical models used (including the parametrisation of turbulence and vertical resolution near the tropopause). Also, there could be an inherent difference between the PV tracer method and the Lagrangian PV diagnostics method, leading to these different signals from PV changes due to turbulence.

Addressing this question fully would require a detailed comparison between the two methodologies using the same data and model, which is beyond the scope of the current study. Nevertheless, given the good agreement between the predictions from the idealised quasi-two-dimensional framework and the dedicated IFS simulation, the tripole pattern of PV tendency due to turbulence should arise if the assumptions of the framework and conditions discussed in Sect. 4.3 are justified.



640 7.2 Non-advective PV flux due to turbulence in environments with instability

The divergent flux from the turbulent layer, which is the basis of the tripole pattern discussed, is, as discussed in Sect. 4.3, expected for most situations with a statically and symmetrically stable flow (i.e., $\frac{\partial \theta}{\partial z} > 0$ and $Q > 0$). While this stable environment is probably the most common situation, one may also be interested in the effect of turbulence in regions with negative PV values. In particular, there are indications from previous studies (Oertel, 2020) that turbulence may be the dominant process in
645 dissipating the negative PV values, which makes this question relevant.

If we revisit Eq. (18) and continue the derivation for regions with negative PV, the non-advective PV flux can converge to the turbulent layer (more details in Appendix B2). Turbulence may thus dissipate negative PV. Nevertheless, as already pointed out in Sect. 3.2, a fundamental assumption of the derivation is the existence of a coherent direction. Since negative PV regions are unstable and less likely to develop into large and coherent structures, the applicability of this assumption is questionable.

650 One should also note that the derivation in Appendix B2 assumes that the entire region of interest has either positive or negative PV values. Regions where PV values are transitioning from positive to negative are hence technically beyond the scope of this derivation. However, clues obtained from analysing selected regions in our IFS simulation at the interface of positive and negative PV (not shown) suggest that the tripole pattern prevails in these regions, indicating that fluxes as predicted by the framework may also apply to these bordering cases. Nevertheless, further investigation is required to confirm if there is a
655 systematic effect of turbulence in regions with negative PV.

7.3 Dependence on the parametrisation of turbulence

In this study, turbulent fluxes are described by the flux-gradient theory, which serves as the basis of all other derived results. The flux-gradient theory is chosen in the derivation as it is a common and simple approach adopted in numerical weather forecasting models to describe turbulent fluxes in the free atmosphere, including the UTLS. The applicability of the results in describing PV
660 modification by turbulence in reality then depends on whether this diffusion-like approach accurately summarises the overall effect of turbulence at the scales concerned.

Assuming the flux-gradient theory is a good approximation, the results obtained from the idealised framework also show that the effect of turbulence on PV modification may depend on the relative strength of turbulent heat and momentum fluxes. As shown in Sect. 4, there is a counteracting effect of turbulent heat and momentum transfer on PV tendencies and the magnitudes
665 of the heat and momentum tendencies ($\dot{\theta}$, $\dot{u}$, $\dot{v}$) may decide if the non-advective PV flux is convergent or divergent towards the turbulent layer (see Eq. 20). Therefore, the ratio of the magnitudes of the heat and momentum transfer terms, which in turn has a dependence on the turbulent Prandtl number $Pr_t = \frac{K_m}{K_h}$, may also be important in determining the qualitative behaviour, though only in rare cases. Previous numerical studies also demonstrated that the magnitudes of the PV changes are dependent on Pr_t (Gidel and Shapiro, 1979), but some studies concluded this to be a minor effect (Hartjensstein, 2000).

670 Verification of the turbulence parametrisation scheme in numerical models with observational data is hence desirable to ensure that the PV modification by turbulence is accurately represented. This would also be important for practical numerical weather prediction, as the sharpness of the tropopause (i.e., the PV gradient), which is influenced by the non-conservative



processes, is related to systematic forecast errors (Gray et al., 2014), indicating that a correct representation of turbulence in the UTLS is essential for the forecast quality. Comparison to measurements by research aircraft may provide a viable means of verification.

7.4 Relevance in different flow situations

One final but important aspect that deserves further discussion concerns the focus on the upper-level jet-front system in the results presented. To study the effect of turbulence on PV modification, the upper-level jet is a natural choice of weather system to begin with as its associated high vertical wind shear has long been recognised as a major source of turbulence in the UTLS, or specifically of clear-air turbulence (e.g., Bannon, 1952; Chambers, 1955). Studies have also revealed that turbulence occurs near upper-level fronts (e.g., Lane et al., 2004; Koch et al., 2005) and tropopause folds (e.g., Lee and Chun, 2018; Rodriguez Imazio et al., 2022). Therefore, we may expect to find the most prominent effects from turbulence on PV in an upper-level jet-front system.

The results of this study are indeed clear in demonstrating that turbulence may modify PV in the UTLS coherently on large scales. The upper-level jet not only provides the coherent direction in the flow field that allows the emergence of elongated bands of instantaneous PV tendencies but also guides air parcels to accumulate consistent PV changes as they flow along the jet axis, leading to the formation of highly coherent APV bands. The possibility of turbulence inducing coherent PV modification near the upper-level jet is of particular importance as the jet serves as the waveguide of large-scale Rossby waves. Therefore, such changes in the PV field potentially affect the propagation of these waves (Harvey et al., 2016). Furthermore, the PV modification by turbulence below the jet is found to dissipate the tropopause fold in the simulation, which points to a linkage with STE, as noted by other studies as well (e.g., Shapiro, 1980; Spreitzer et al., 2019).

However, the upper-level jet-front system is seemingly a tailor-made example for investigating the effect of turbulence on PV modification. Still, one may ask whether the results are also relevant or applicable to other flow situations, especially those that are more complicated. Although the idealised framework introduced is inspired by the situation associated with an upper-level jet, any flow situation that generates strong vertical shear and thus turbulence along a coherent direction (justifying the quasi-two-dimensional approximation) would, in principle, result in the elongate PV tendency bands. Yet, a consistent accumulation of PV changes would have to be enabled by the flow field as well in order to have a coherent and systematic effect on the dynamics at larger scales. We will explore one such flow situation in Part 2 of this study, which involves the outflow from a warm conveyor belt reaching the upper troposphere. As will be illustrated in Part 2, coherent PV modification is also induced by turbulence in this flow situation, but achieved through a considerably more abstruse pathway. While the details will only be presented in Part 2, we can claim here already that the upper-level jet-front system is not the only weather system or flow situation that allows coherent PV modification by turbulence, albeit it is the most straightforward one in demonstrating this possibility.



8 Conclusions

705 This study investigates the PV modification by turbulence in the UTLS with two complementary tools, an analytical idealised quasi-two-dimensional framework and diagnostics based on a dedicated IFS simulation. The idealisations employed in the analytical framework elucidate the underlying relationships between turbulent fluxes and PV modification and the basic fundamental assumptions provide the possibility to generalise the results. The IFS simulation, on the other hand, allows for justifying the relevance of the idealised framework to realistic flow situations and examining the pathway through which the accumulated PV modification by turbulence becomes significant in complex atmospheric flows. The combined results from this novel approach reveal that turbulence can systematically and coherently modify PV and they provide a mechanistic understanding of this behaviour in upper-level jet-front systems.

The idealised framework is based on two fundamental assumptions, namely the flux-gradient theory description of turbulent fluxes and the existence of a coherent direction that enables the quasi-two-dimensional approximation. While the first is a common assumption for turbulence in the UTLS, the latter is flow-dependent but not restrictive, as is demonstrated in the example of the upper-level jet-front system. Three characteristics of PV modification by turbulence are then derived and summarised in Sect. 4, including their corresponding required conditions. The most important one is undoubtedly the divergent non-advective PV flux due to turbulence from the turbulent layer in most situations when the environment is statically and symmetrically stable. When considering the vertical section across a simulated upper-level jet-front system in Sect. 5, these divergent fluxes occur prominently and show remarkable agreement with the theoretically postulated PV tendency tripole centred at the shear zones. These analyses, therefore, may serve as a mechanistic explanation for the signals found for the turbulence-induced PV modification in previous studies (e.g., Hartjenstein, 2000; Spreitzer et al., 2019). The idealised framework not only advances our understanding of how turbulence modifies PV, but also provides clear indications of the conditions under which the results may be applied, offering broad generalisability to different flow situations.

725 While the instantaneous behaviour of turbulence-induced PV modification is addressed by the idealised framework, the trajectory analysis conducted with the IFS simulation offers a Lagrangian perspective to understand the accumulation of the effect of turbulence on PV modification. With the reverse domain filling method, the most prominent material PV changes near the upper-level jet-front system are attributed to turbulence. The accumulated PV changes due to turbulence also feature elongated bands along the upper-level jet, closely resembling the spatial pattern observed in the instantaneous PV tendency field. The vertical profiles along selected trajectories further reveal that air parcels remain consistently at a constant location relative to the turbulence-induced PV tendency tripole when advected along the upper-level jet, thereby enabling the emergence of coherent accumulated PV changes in the UTLS. This example demonstrates that turbulence can induce significant and coherent PV modification in the tropopause region, possibly influencing Rossby wave dynamics (e.g., Harvey et al., 2016) and leading to STE (e.g., Shapiro, 1980; Spreitzer et al., 2019).

735 The integrated results also highlight the multifaceted role of the upper-level jet-front system in facilitating the systematic PV modification by turbulence, as summarised schematically in Fig. 10. With the upper-level jet-front system being a coherent flow structure, it first provides a horizontal direction with small variations, which is along the jet axis. This serves as the coherent

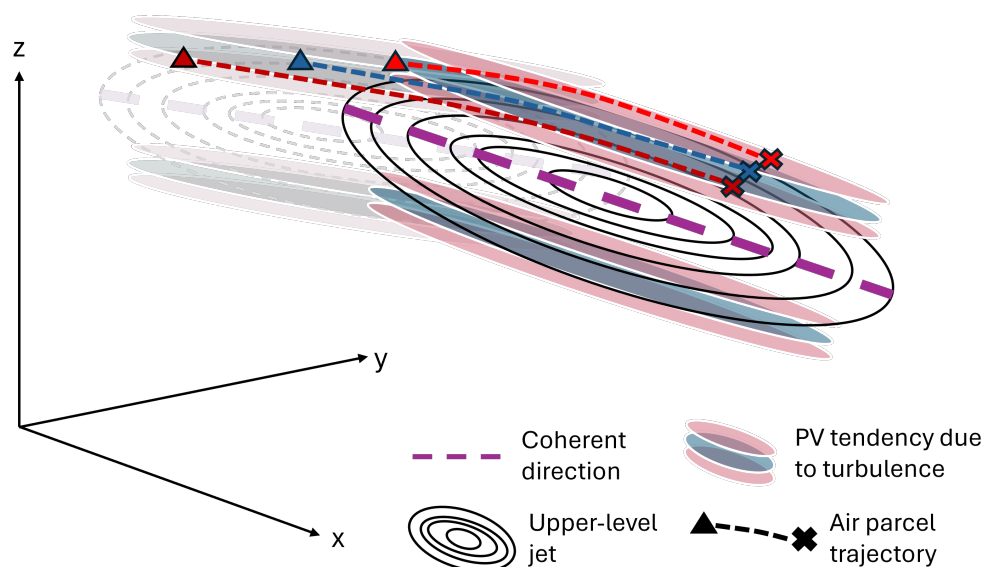


Figure 10. Schematic illustration of PV modification by turbulence associated with an upper-level jet-front system (with translucent components indicating the system at an earlier time). With tripolar PV tendency bands developed in the shear zones above and below the jet core along the coherent direction (jet axis), air parcels accumulate PV changes consistently as they are advected along the upper-level jet from their previous positions (triangles) to their current positions (crosses), resulting in coherent and prominent PV modification due to turbulence.

direction required for the quasi-two-dimensional framework, which predicts the divergent non-advective PV flux from the turbulent layer and the formation of the elongated tripolar PV tendency bands. Apart from organising the PV tendency into structured tripoles, the upper-level jet further guides air parcels to travel steadily along the jet axis and accumulate turbulence-induced PV changes in a fairly uniform way over several hours. Consequently, it permits the accumulation of the instantaneous PV tendency due to turbulence and the resultant material PV changes may influence the dynamics in the UTLS region. The upper-level jet-front system thus provides the coherence required in both the spatial and temporal dimensions for significant PV modification by turbulence.

While a high correspondence is present between the idealised framework and the simulated upper-level jet-front system, it is intriguing to explore whether the results obtained are still valid in more three-dimensional and dynamically evolving flow situations. This will be the subject of Part 2 of this study, which aims at corroborates the current findings in another simulation involving a warm conveyor belt outflow, though with an unexpected and very different pathway. The results also invite verification with observational data to validate or improve the representation of turbulence in numerical weather prediction models and thus the quality of the forecasts. By establishing a more thorough mechanistic understanding of PV modification by turbulence, this work may serve as the foundation of future investigations, especially on the dynamical impacts of these turbulence-induced PV changes in the UTLS region.



Code and data availability. Trajectory calculations are performed using the LAGRANTO tool v2.0 (Sprenger and Wernli, 2015), which is available at <https://iacweb.ethz.ch/staff/sprenger/lagranto/>. Other data are available upon request to the authors.

755 Appendix A: Simplification of the PV modification equation with the quasi-two-dimensional approximation

Starting from Eq. (2b), we may expand the right-hand side into its component form. We take $\mathbf{F} = (\dot{u}, \dot{v}, 0)$ since there is no vertical wind tendency $\dot{w}$ due to parametrisation in the IFS and it should generally be negligible compared to the horizontal wind tendencies $\dot{u}$ and $\dot{v}$. Substituting this form of $\mathbf{F}$ into Eq. (2b), it yields:

$$\begin{aligned} \frac{DQ}{Dt} &= -\alpha \nabla \cdot \left(-\zeta_a \dot{\theta} + \nabla \theta \times \mathbf{F} \right) \\ &= \alpha \left\{ -\frac{\partial}{\partial x} \left[\dot{\theta} \left(\frac{\partial v}{\partial z} - \frac{\partial w}{\partial y} \right) \right] - \frac{\partial}{\partial y} \left[\dot{\theta} \left(\frac{\partial w}{\partial x} - \frac{\partial u}{\partial z} \right) \right] - \frac{\partial}{\partial z} \left[\dot{\theta} \left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} \right) \right] \right. \\ &\quad \left. + e \frac{\partial \dot{\theta}}{\partial y} + f \frac{\partial \dot{\theta}}{\partial z} - \frac{\partial}{\partial x} \left(-\dot{v} \frac{\partial \theta}{\partial z} \right) - \frac{\partial}{\partial y} \left(\dot{u} \frac{\partial \theta}{\partial z} \right) - \frac{\partial}{\partial z} \left(\dot{v} \frac{\partial \theta}{\partial x} - \dot{u} \frac{\partial \theta}{\partial y} \right) \right\} \\ &\simeq \alpha \left\{ -\frac{\partial}{\partial x} \left(\dot{\theta} \frac{\partial v}{\partial z} \right) - \frac{\partial}{\partial y} \left(-\dot{\theta} \frac{\partial u}{\partial z} \right) - \frac{\partial}{\partial z} \left[\dot{\theta} \left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} - f \right) \right] \right. \\ &\quad \left. - \frac{\partial}{\partial x} \left(-\dot{v} \frac{\partial \theta}{\partial z} \right) - \frac{\partial}{\partial y} \left(\dot{u} \frac{\partial \theta}{\partial z} \right) - \frac{\partial}{\partial z} \left(\dot{v} \frac{\partial \theta}{\partial x} - \dot{u} \frac{\partial \theta}{\partial y} \right) \right\}, \end{aligned} \quad (\text{A1})$$

760 where $e = 2\Omega \cos \phi$ and $f = 2\Omega \sin \phi$ are the Coriolis parameters, with ϕ being latitude. The last line is obtained by neglecting the horizontal derivatives of w and $e \frac{\partial \dot{\theta}}{\partial y}$, as they are orders of magnitude smaller than the vertical derivatives of u or v and $f \frac{\partial \dot{\theta}}{\partial z}$, respectively. From Eq. (A1), if one applies the quasi-two-dimensional approximation and neglects all terms associated with derivatives in the x-direction, Eq. (11) is obtained.

Appendix B: Turbulence-induced non-advective PV flux

765 B1 Divergent flux from isotachs near the turbulent layer

In Sect. 4.3, we identify “convergent” or “divergent” non-advective PV flux towards isentropes and the isopleths of m near the turbulent layer by determining the signs of the scalar products of $\mathbf{H} + \mathbf{M}$ with the $\nabla \theta$ and ∇m (Eq. 17). We concluded that if the region is statically stable ($\frac{\partial \theta}{\partial z} > 0$) and has positive PV ($Q > 0$), the non-advective PV flux is always diverging from isentropes and isopleths of m . As stated there, the flux is also diverging from isotachs most of the time in such a region, but
770 with some rare exceptions. Since the complete derivation is lengthy, the details are only presented here.

We again start with a scalar product, but between $\mathbf{H} + \mathbf{M}$ and ∇u for isotachs:

$$(\mathbf{H} + \mathbf{M}) \cdot \nabla u = -\dot{u} \left(\frac{\partial \theta}{\partial y} \frac{\partial u}{\partial z} - \frac{\partial \theta}{\partial z} \frac{\partial u}{\partial y} \right) - \dot{\theta} f \frac{\partial u}{\partial z}, \quad (\text{B1})$$

which is the same as Eq. (18). Since ∇u points towards the high wind speed, if the scalar product is positive on the side with higher wind speed and negative on the side with lower wind speed, the fluxes are diverging from the isotachs. Considering the



Table B1. Sign of different quantities above and below the turbulent layer.

	$(\mathbf{H} + \mathbf{M}) \cdot \nabla u$ (divergent)	$(\mathbf{H} + \mathbf{M}) \cdot \nabla u$ (convergent)	$\dot{u}$	$\dot{\theta}$
Above	$+\frac{\partial u}{\partial z}$	$-\frac{\partial u}{\partial z}$	$-\frac{\partial u}{\partial z}$	$-\frac{\partial \theta}{\partial z}$
Below	$-\frac{\partial u}{\partial z}$	$+\frac{\partial u}{\partial z}$	$+\frac{\partial u}{\partial z}$	$+\frac{\partial \theta}{\partial z}$

vertical direction, it means the non-advective PV flux is divergent if the scalar product has the same sign as $+\frac{\partial u}{\partial z}$ above and that of $-\frac{\partial u}{\partial z}$ below the turbulent layer. The opposite holds for convergent fluxes, and these statements are summarised in the first two columns of Table B1.

Moreover, from the flux-gradient theory, $\dot{u}$ has the same sign as $-\frac{\partial u}{\partial z}$ above the turbulent layer and as $+\frac{\partial u}{\partial z}$ below. The sign of $\dot{\theta}$ is likewise related to $\mp \frac{\partial \theta}{\partial z}$ above and below the turbulent layer, and these are listed in the last two columns of Table B1. With this look-up table, we can easily check whether the flux is divergent or convergent by evaluating the signs of the right-hand side of Eq. (B1) above and below the turbulent layer.

We can first check signs of the second term in Eq. (B1), $-\dot{\theta} f \frac{\partial u}{\partial z}$, which originates from $\mathbf{H} \cdot \nabla u$. For statically stable conditions in the Northern Hemisphere, $\frac{\partial \theta}{\partial z} > 0$ and $f > 0$. Inspecting Table B1, we can see that this term has the sign of $+\frac{\partial u}{\partial z}$ above and that of $-\frac{\partial u}{\partial z}$ below the turbulent layer. This term contributes to the divergence of the flux and $\mathbf{H}$ is thus always divergent from the isotachs.

Therefore, the total non-advective PV flux, $\mathbf{H} + \mathbf{M}$, can only be convergent if (i) $\mathbf{M}$ is convergent and (ii) $\mathbf{M} \cdot \nabla u$ is larger in magnitude compared to $\mathbf{H} \cdot \nabla u$. For (i) $\mathbf{M}$ to be convergent, the first term in Eq. (B1), $-\dot{u} \left(\frac{\partial \theta}{\partial y} \frac{\partial u}{\partial z} - \frac{\partial \theta}{\partial z} \frac{\partial u}{\partial y} \right)$, should have the sign of $\mp \frac{\partial u}{\partial z}$ above and below the turbulent layer. By inspecting Table B1, this implies that $\frac{\partial \theta}{\partial y} \frac{\partial u}{\partial z} - \frac{\partial \theta}{\partial z} \frac{\partial u}{\partial y}$ must be negative. Furthermore, since the region has positive PV ($Q > 0$), Eq. (12a) additionally sets a lower bound to this quantity, which leads to the following condition:

$$0 > \left(\frac{\partial \theta}{\partial y} \frac{\partial u}{\partial z} - \frac{\partial \theta}{\partial z} \frac{\partial u}{\partial y} \right) > -f \left(\frac{\partial \theta}{\partial z} \right). \quad (\text{B2})$$

For (ii) to be satisfied:

$$\left| \dot{u} \left(\frac{\partial \theta}{\partial y} \frac{\partial u}{\partial z} - \frac{\partial \theta}{\partial z} \frac{\partial u}{\partial y} \right) \right| > \left| \dot{\theta} f \frac{\partial u}{\partial z} \right|. \quad (\text{B3})$$

Convergent flux is possible only if the two conditions listed are satisfied simultaneously. This is rarely realised because Eq. (B2) turns out very restrictive. To show this more clearly, we rearrange Eq. (B2):

$$\begin{cases} \frac{\partial u}{\partial y} / \frac{\partial u}{\partial z} > \frac{\partial \theta}{\partial y} / \frac{\partial \theta}{\partial z} > \left(\frac{\partial u}{\partial y} - f \right) / \frac{\partial u}{\partial z} & \text{if } \frac{\partial u}{\partial z} > 0 \\ \frac{\partial u}{\partial y} / \frac{\partial u}{\partial z} < \frac{\partial \theta}{\partial y} / \frac{\partial \theta}{\partial z} < \left(\frac{\partial u}{\partial y} - f \right) / \frac{\partial u}{\partial z} & \text{if } \frac{\partial u}{\partial z} < 0. \end{cases} \quad (\text{B4})$$

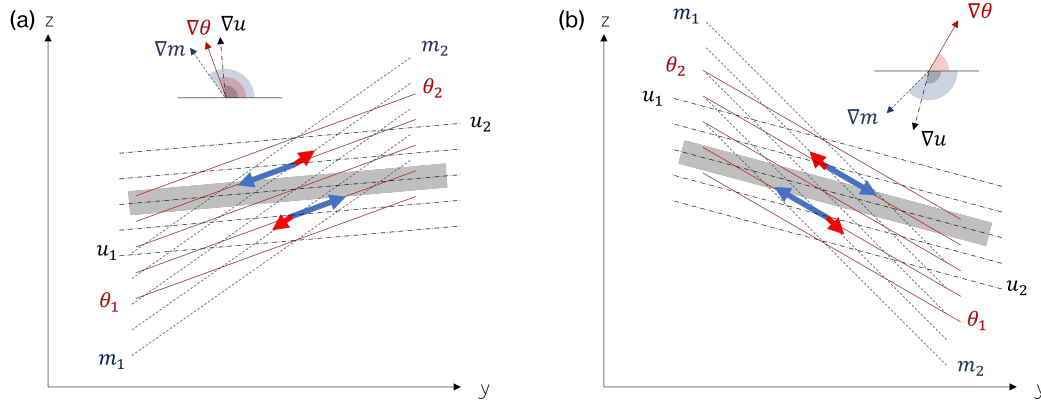


Figure B1. Examples of convergent total non-advective PV flux due to turbulence $\mathbf{H} + \mathbf{M}$, where $\mathbf{H}$ and $\mathbf{M}$ are represented by red and blue arrows, respectively, in the yz plane for stable configurations with (a) $\frac{\partial u}{\partial z} > 0$ and (b) $\frac{\partial u}{\partial z} < 0$. The turbulent layer (grey shading) is tilted and assumed to be aligned with isotachs (black dash-dotted lines, with $u_2 > u_1$). The isentropes (red solid lines) and isopleths of m (blue dashed lines) are plotted with $\theta_2 > \theta_1$ and $m_2 > m_1$. The directions of $\nabla\theta$, ∇m and ∇u are indicated at the top and their angles from the y -axis are indicated by corresponding shadings. $\mathbf{M}$ converges towards the isotachs in the turbulent layer only when the slope of the isentropes is intermediate to the slope of the isotachs and isopleths of m (see text for explanation). Convergent total non-advective PV flux due to turbulence is then possible only if $\mathbf{H}$ also has a small enough magnitude to satisfy Eq. (B3).

The inequalities can be interpreted geometrically as conditions on the angles of $\nabla\theta$, ∇m and ∇u from the horizontal axis and example flow situations satisfying these conditions are illustrated in Fig. B1. If we denote the angles from the y -axis to the three vectors as δ_θ , δ_m and δ_u , respectively (indicated by shadings in Fig. B1), the first line of inequality Eq. (B4) states that $\cot \delta_u > \cot \delta_\theta > \cot \delta_m$. As $\frac{\partial \theta}{\partial z}$ and $\frac{\partial u}{\partial z}$ are both positive, all the angles are within the range $(0, \pi)$. The cotangent function is monotonically decreasing in this domain and therefore $\delta_u < \delta_\theta < \delta_m$, which is fulfilled in Fig. B1a. Similarly, the second line of inequality Eq. (B4) gives $\cot \delta_u < \cot \delta_\theta < \cot \delta_m$. However, as $0 < \delta_\theta < \pi$ while $-\pi < \delta_{m,u} < 0$ in this case, $\cot \delta_\theta$ is mapped to $\cot(\delta_\theta - \pi)$ using the periodicity of the cotangent function. Therefore, as the cotangent function is again monotonically decreasing in $(-\pi, 0)$, $\delta_u > \delta_\theta - \pi > \delta_m$, it is satisfied in Fig. B1b.

As a result, the total non-advective PV flux due to turbulence can be convergent towards the isotachs in the turbulent layer only if the slope of isentropes is within the range set by the slopes of the isotachs and the isopleths of m . In addition, the condition in Eq. (B3) has to be fulfilled at the same time in order to have a convergent non-advective PV flux due to turbulence. All other configurations have a divergent flux from the isotachs in the turbulent layer (or parallel to the isotachs in limiting cases). The range of slopes of isentropes allowed for a convergent flux depends on the angle between the slopes of isotachs and isopleths of m , or equivalently the angle between the relative vorticity ζ and the absolute vorticity ζ_a vectors, which in turn depends on the ratio $f/\frac{\partial u}{\partial z}$. The stronger the vertical wind shear in a region, the smaller the range for the allowed slopes of isentropes for convergent flux. Consequently, the total non-advective PV flux due to turbulence should be divergent from the isotachs near the turbulent layer in most situations if the region is statically stable and has positive PV.



B2 Flux divergence in regions with instability

Throughout Sect. 4.3 and Appendix B1, we focused on the statically stable situation with PV being positive (i.e., $\frac{\partial \theta}{\partial z} > 0$ and $Q > 0$). The resultant non-advective PV flux is found to be divergent from the layer with maximum turbulent fluxes, unless conditions in Eq. (B2) and (B3) are satisfied. While the focus was on stable flow conditions, a pertinent question would be the behaviour of the non-advective PV flux in regions with negative PV, especially as turbulence was suggested to be a process that dissipates negative PV in the UTLS (e.g., Oertel, 2020). To explore the unstable cases, we again extend our analysis of the scalar product $(\mathbf{H} + \mathbf{M}) \cdot \nabla u$ and utilise the look-up table (Table B1) to determine the conditions for the non-advective PV flux being divergent or convergent.

We first start with statically unstable situations with negative PV (i.e., $\frac{\partial \theta}{\partial z} < 0$ and $Q < 0$). The heat transfer term $-\dot{\theta} f \frac{\partial u}{\partial z}$ will now have the sign of $-\frac{\partial u}{\partial z}$ above the layer and that of $+\frac{\partial u}{\partial z}$ below the layer, given $f > 0$ in the Northern Hemisphere. From Table B1, the heat transfer term is convergent. Therefore, to have a divergent non-advective PV flux, the momentum transfer term $-\dot{u} \left(\frac{\partial \theta}{\partial y} \frac{\partial u}{\partial z} - \frac{\partial \theta}{\partial z} \frac{\partial u}{\partial y} \right)$ must be divergent and outweigh the heat transfer term. It results in exactly the same conditions as stated in Eq. (B2) and (B3), but for divergent fluxes this time. Therefore, similar to the conclusions in Appendix B1, the total non-advective PV flux due to turbulence mostly converges towards the turbulent layer, except for the occasions where both Eq. (B2) and (B3) are satisfied.

We continue to examine the situations with negative PV that are statically stable (i.e., $\frac{\partial \theta}{\partial z} > 0$ and $Q < 0$). In this configuration, the heat transfer term is divergent because it has the sign of $+\frac{\partial u}{\partial z}$ above the layer and that of $-\frac{\partial u}{\partial z}$ below the layer. Given that PV is negative (cf. Eq. 12a):

$$\nabla \theta \cdot \zeta_a = \frac{\partial \theta}{\partial y} \frac{\partial m}{\partial z} - \frac{\partial \theta}{\partial z} \frac{\partial m}{\partial y} < 0 \quad (\text{B5})$$

When rearranged, it gives,

$$\frac{\partial \theta}{\partial y} \frac{\partial u}{\partial z} - \frac{\partial \theta}{\partial z} \frac{\partial u}{\partial y} < -f \frac{\partial \theta}{\partial z} \quad (\text{B6})$$

Since the region is statically stable, the right-hand side of Eq. (B6) is always negative. Checking Table B1 for the signs of $\dot{u}$, the momentum transfer term is always convergent. Therefore, the total non-advective PV flux due to turbulence diverges if the heat transfer term dominates, and converges if the momentum transfer term dominates.

The remaining situations yet to be explored are those being statically unstable with positive PV (i.e., $\frac{\partial \theta}{\partial z} < 0$ and $Q > 0$). They should be very rare in the atmosphere, but they are included here for completeness. Going through the same exercise, one can conclude that the heat transfer term is always convergent while the momentum transfer term is always divergent, as PV is positive. As a result, the total non-advective PV flux converges if the heat transfer term dominates, and diverges if the momentum transfer term dominates.

The results are tabulated in Table B2. While we may conclude that the total non-advective PV flux due to turbulence is mostly divergent and convergent, respectively, for the first two situations, the results are inconclusive for the remaining two cases. The conclusion for the latter two situations depends on the relative magnitudes of the heat transfer and momentum transfer terms, which in turn depend on the background gradients and the turbulence parametrisation scheme (e.g., the turbulent Prandtl



Table B2. Divergence of non-advective PV flux with respect to the turbulent layer in different situations.

Situation	Divergence of non-advective PV flux
$\frac{\partial \theta}{\partial z} > 0, Q > 0$	Convergent only if Eq. (B2) and (B3) are satisfied Divergent otherwise (i.e., in most situations)
$\frac{\partial \theta}{\partial z} < 0, Q < 0$	Divergent only if Eq. (B2) and (B3) are satisfied Convergent otherwise (i.e., in most situations)
$\frac{\partial \theta}{\partial z} > 0, Q < 0$	Convergent if Eq. (B3) is satisfied Divergent otherwise
$\frac{\partial \theta}{\partial z} < 0, Q > 0$	Divergent if Eq. (B3) is satisfied Convergent otherwise

number $Pr_t = \frac{K_m}{K_h}$). Moreover, as these unstable configurations may be restricted spatially, the fundamental assumption of having a coherent direction may not be justified. Consequently, the results obtained here for the unstable situations should only be treated as a theoretical extension of the derivation in Sect. 4.3 and Appendix B1, with the applicability to the real atmosphere remaining unknown.

Author contributions. MHFL and MS formulated and designed the study. RF implemented the changes to the IFS source code for this study. MHFL performed the simulation, data analysis and wrote the manuscript. MS, HJ and HW contributed significantly to the interpretation of the results and gave feedback on the manuscript.

Competing interests. At least one of the (co-)authors is a member of the editorial board of Weather and Climate Dynamics.

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References

- Attinger, R., Spreitzer, E., Boettcher, M., Forbes, R., Wernli, H., and Joos, H.: Quantifying the role of individual diabatic processes for the formation of PV anomalies in a North Pacific cyclone, *Quart. J. Roy. Meteor. Soc.*, 145, 2454–2476, <https://doi.org/10.1002/QJ.3573>, 2019.
- Attinger, R., Spreitzer, E., Boettcher, M., Wernli, H., and Joos, H.: Systematic assessment of the diabatic processes that modify low-level potential vorticity in extratropical cyclones, *Weather Clim. Dynam.*, 2, 1073–1091, <https://doi.org/10.5194/WCD-2-1073-2021>, 2021.
- 865 Bannon, J. K.: Weather systems associated with some occasions of severe turbulence at high altitude, *Meteorol. Mag.*, 81, 97–101, available at https://digital.nmla.metoffice.gov.uk/IO_19362a02-cf23-4875-a63e-bfd8dbcb4118/, 1952.
- Bechtold, P., Forbes, R., Sandu, I., Lang, S., and Ahlgrim, M.: A major moist physics upgrade for the IFS, *ECMWF Newsletter*, 164, 24–32, <https://doi.org/10.21957/3gt59vx1pb>, 2020.
- Beljaars, A. C. M., Brown, A. R., and Wood, N.: A new parametrization of turbulent orographic form drag, *Quart. J. Roy. Meteor. Soc.*, 130, 1327–1347, <https://doi.org/10.1256/QJ.03.73>, 2004.
- 870 Chagnon, J. M. and Gray, S. L.: Horizontal potential vorticity dipoles on the convective storm scale, *Quart. J. Roy. Meteor. Soc.*, 135, 1392–1408, <https://doi.org/10.1002/QJ.468>, 2009.
- Chagnon, J. M. and Gray, S. L.: A diabatically generated potential vorticity structure near the extratropical tropopause in three simulated extratropical cyclones, *Mon. Wea. Rev.*, 143, 2337–2347, <https://doi.org/10.1175/MWR-D-14-00092.1>, 2015.
- 875 Chagnon, J. M., Gray, S. L., and Methven, J.: Diabatic processes modifying potential vorticity in a North Atlantic cyclone, *Quart. J. Roy. Meteor. Soc.*, 139, 1270–1282, <https://doi.org/10.1002/QJ.2037>, 2013.
- Chambers, E.: Clear air turbulence and civil jet operations, *J. R. Aeronaut. Soc.*, 59, 613–628, <https://doi.org/10.1017/S036839310011692X>, 1955.
- Crezee, B., Joos, H., and Wernli, H.: The microphysical building blocks of low-level potential vorticity anomalies in an idealized extratropical cyclone, *J. Atmos. Sci.*, 74, 1403–1416, <https://doi.org/10.1175/JAS-D-16-0260.1>, 2017.
- 880 ECMWF: IFS Documentation CY47R3 - Part IV Physical processes, ECMWF, <https://doi.org/10.21957/eyrpir4vj>, 2021.
- Eliassen, A. and Kleinschmidt, E.: *Dynamic meteorology*, p. 1–154, Springer Berlin Heidelberg, Berlin, Heidelberg, ISBN 978-3-642-45881-1, https://doi.org/10.1007/978-3-642-45881-1_1, 1957.
- Ertel, H.: Ein neuer hydrodynamischer Erhaltungssatz, *Die Naturwissenschaften*, 30, 543–544, <https://doi.org/10.1007/BF01475602/METRICS>, 1942.
- 885 Forbes, R., Laloyaux, P., and Rodwell, M.: IFS upgrade improves moist physics and use of satellite observations, *ECMWF Newsletter*, 169, 17–24, <https://doi.org/10.21957/m3805gf17r>, 2021.
- Gidel, L. T. and Shapiro, M. A.: The role of clear air turbulence in the production of potential vorticity in the vicinity of upper tropospheric jet stream-frontal systems, *J. Atmos. Sci.*, 36, 2125 – 2138, [https://doi.org/10.1175/1520-0469\(1979\)036<2125:TROCAT>2.0.CO;2](https://doi.org/10.1175/1520-0469(1979)036<2125:TROCAT>2.0.CO;2), 1979.
- 890 Gray, S. L.: Mechanisms of midlatitude cross-tropopause transport using a potential vorticity budget approach, *J. Geophys. Res.-Atmos.*, 111, <https://doi.org/10.1029/2005JD006259>, 2006.
- Gray, S. L., Dunning, C. M., Methven, J., Masato, G., and Chagnon, J. M.: Systematic model forecast error in Rossby wave structure, *Geophys. Res. Lett.*, 41, 2979–2987, <https://doi.org/10.1002/2014GL059282>, 2014.
- Hartjenstein, G.: Diffusive decay of tropopause folds and the related cross-tropopause mass flux, *Mon. Wea. Rev.*, 128, 2958 – 2966, [https://doi.org/10.1175/1520-0493\(2000\)128<2958:DDOTFA>2.0.CO;2](https://doi.org/10.1175/1520-0493(2000)128<2958:DDOTFA>2.0.CO;2), 2000.
- 895



- Harvey, B., Methven, J., Sanchez, C., and Schäfler, A.: Diabatic generation of negative potential vorticity and its impact on the North Atlantic jet stream, *Quart. J. Roy. Meteor. Soc.*, 146, 1477–1497, <https://doi.org/10.1002/QJ.3747>, 2020.
- Harvey, B. J., Methven, J., and Ambaum, M. H.: Rossby wave propagation on potential vorticity fronts with finite width, *J. Fluid Mech.*, 794, 775–797, <https://doi.org/10.1017/JFM.2016.180>, 2016.
- 900 Haynes, P. H. and McIntyre, M. E.: On the evolution of vorticity and potential vorticity in the presence of diabatic heating and frictional or other Forces, *J. Atmos. Sci.*, 44, 828–841, [https://doi.org/10.1175/1520-0469\(1987\)044<0828:oteova>2.0.co;2](https://doi.org/10.1175/1520-0469(1987)044<0828:oteova>2.0.co;2), 1987.
- Haynes, P. H. and McIntyre, M. E.: On the conservation and impermeability theorems for potential vorticity, *J. Atmos. Sci.*, 47, 2021–2031, [https://doi.org/10.1175/1520-0469\(1990\)047<2021:OTCAIT>2.0.CO;2](https://doi.org/10.1175/1520-0469(1990)047<2021:OTCAIT>2.0.CO;2), 1990.
- Holton, J. R. and Hakim, G. J.: Chapter 8 - The planetary boundary layer, in: *An introduction to dynamic meteorology*, edited by Holton, J. R. and Hakim, G. J., p. 255–277, Academic Press, Boston, fifth edition edn., ISBN 978-0-12-384866-6, <https://doi.org/10.1016/B978-0-12-384866-6.00008-8>, 2013.
- 905 Hoskins, B. J., McIntyre, M. E., and Robertson, A. W.: On the use and significance of isentropic potential vorticity maps, *Quart. J. Roy. Meteor. Soc.*, 111, 877–946, <https://doi.org/10.1002/QJ.49711147002>, 1985.
- Joos, H. and Wernli, H.: Influence of microphysical processes on the potential vorticity development in a warm conveyor belt: A case-study with the limited-area model COSMO, *Quart. J. Roy. Meteor. Soc.*, 138, 407–418, <https://doi.org/10.1002/qj.934>, 2012.
- 910 Keyser, D. and Shapiro, M. A.: A review of the structure and dynamics of upper-level frontal zones., *Mon. Wea. Rev.*, 114, 452–499, [https://doi.org/10.1175/1520-0493\(1986\)114<0452:AROTSA>2.0.CO;2](https://doi.org/10.1175/1520-0493(1986)114<0452:AROTSA>2.0.CO;2), 1986.
- Koch, S. E., Jamison, B. D., Lu, C., Smith, T. L., Tollerud, E. I., Girz, C., Wang, N., Lane, T. P., Shapiro, M. A., Parrish, D. D., and Cooper, O. R.: Turbulence and gravity waves within an upper-level front, *J. Atmos. Sci.*, 62, 3885–3908, <https://doi.org/10.1175/JAS3574.1>, 2005.
- 915 Köhler, M., Ahlgrim, M., and Beljaars, A.: Unified treatment of dry convective and stratocumulus-topped boundary layers in the ECMWF model, *Quart. J. Roy. Meteor. Soc.*, 137, 43–57, <https://doi.org/10.1002/QJ.713>, 2011.
- Lamarque, J.-F. and Hess, P. G.: Cross-tropopause mass exchange and potential vorticity budget in a simulated tropopause folding, *J. Atmos. Sci.*, 51, 2246–2269, [https://doi.org/10.1175/1520-0469\(1994\)051<2246:CTMEAP>2.0.CO;2](https://doi.org/10.1175/1520-0469(1994)051<2246:CTMEAP>2.0.CO;2), 1994.
- Lane, T. P., Doyle, J. D., Plougonven, R., Shapiro, M. A., and Sharman, R. D.: Observations and numerical simulations of inertia-gravity waves and shearing instabilities in the vicinity of a jet stream, *J. Atmos. Sci.*, 61, 2692–2706, <https://doi.org/10.1175/JAS3305.1>, 2004.
- 920 Lee, D. B. and Chun, H. Y.: A numerical study of aviation turbulence encountered on 13 February 2013 over the Yellow Sea between China and the Korean Peninsula, *J. Appl. Meteor. Climatol.*, 57, 1043–1060, <https://doi.org/10.1175/JAMC-D-17-0247.1>, 2018.
- Lee, M. H. F.: Clear-air turbulence - generation, predictability, and feedback in weather systems, Ph.D. thesis, ETH Zurich, <https://doi.org/10.3929/ethz-c-000795586>, 2025.
- 925 Liniger, M. A. and Davies, H. C.: Substructure of a MAP streamer, *Quart. J. Roy. Meteor. Soc.*, 129, 633–651, <https://doi.org/10.1256/QJ.02.28>, 2003.
- Lott, F. and Miller, M. J.: A new subgrid-scale orographic drag parametrization: Its formulation and testing, *Quart. J. Roy. Meteor. Soc.*, 123, 101–127, <https://doi.org/10.1002/QJ.49712353704>, 1997.
- Louis, J.-F., Tiedtke, M., and Geleyn, J.-F.: A short history of the PBL parameterization at ECMWF, in: *Workshop on Planetary Boundary Layer parameterization*, 25–27 November 1981, pp. 59–79, ECMWF, available at <https://www.ecmwf.int/en/elibrary/75473-short-history-pbl-parameterization-ecmwf>, 1982.
- 930 Oertel, A.: Embedded convection in warm conveyor belts, Ph.D. thesis, ETH Zurich, <https://doi.org/10.3929/ETHZ-B-000414750>, 2020.



- Oertel, A., Boettcher, M., Joos, H., Sprenger, M., and Wernli, H.: Potential vorticity structure of embedded convection in a warm conveyor belt and its relevance for large-scale dynamics, *Weather Clim. Dynam.*, 1, 127–153, <https://doi.org/10.5194/wcd-1-127-2020>, 2020.
- 935 Orr, A., Bechtold, P., Scinocca, J., Ern, M., and Janiskova, M.: Improved middle atmosphere climate and forecasts in the ECMWF model through a nonorographic gravity wave drag parameterization, *J. Climate*, 23, 5905–5926, <https://doi.org/10.1175/2010JCLI3490.1>, 2010.
- Price, J. D. and Vaughan, G.: The potential for stratosphere-troposphere exchange in cut-off-low systems, *Quart. J. Roy. Meteor. Soc.*, 119, 343–365, <https://doi.org/10.1002/QJ.49711951007>, 1993.
- Rodriguez Imazio, P., Dörnbrack, A., Urzua, R. D., Rivaben, N., and Godoy, A.: Clear air turbulence observed across a tropopause fold over the Drake Passage—a case study, *J. Geophys. Res.-Atmos.*, 127, e2021JD035 908, <https://doi.org/10.1029/2021JD035908>, 2022.
- 940 Saffin, L., Gray, S. L., Methven, J., and Williams, K. D.: Processes maintaining tropopause sharpness in numerical models, *J. Geophys. Res.-Atmos.*, 122, 9611–9627, <https://doi.org/10.1002/2017JD026879>, 2017.
- Schoeberl, M. R. and Newman, P. A.: A multiple-level trajectory analysis of vortex filaments, *J. Geophys. Res.*, 100, 25 801–25 815, <https://doi.org/10.1029/95JD02414>, 1995.
- 945 Shapiro, M. A.: The role of turbulent heat flux in the generation of potential vorticity in the vicinity of upper-level jet stream systems, *Mon. Wea. Rev.*, 104, 892–906, [https://doi.org/10.1175/1520-0493\(1976\)104<0892:TROTHF>2.0.CO;2](https://doi.org/10.1175/1520-0493(1976)104<0892:TROTHF>2.0.CO;2), 1976.
- Shapiro, M. A.: Turbulent mixing within tropopause folds as a mechanism for the exchange of chemical constituents between the stratosphere and troposphere, *J. Atmos. Sci.*, 37, 994–1004, [https://doi.org/10.1175/1520-0469\(1980\)037<0994:TMWTFA>2.0.CO;2](https://doi.org/10.1175/1520-0469(1980)037<0994:TMWTFA>2.0.CO;2), 1980.
- Spreitzer, E., Attinger, R., Boettcher, M., Forbes, R., Wernli, H., and Joos, H.: Modification of potential vorticity near the tropopause by nonconservative processes in the ECMWF model, *J. Atmos. Sci.*, 76, 1709–1726, <https://doi.org/10.1175/JAS-D-18-0295.1>, 2019.
- 950 Spreitzer, E. J.: Diabatic processes in mid-latitude weather systems - a study with the ECMWF model, Ph.D. thesis, ETH Zurich, <https://doi.org/10.3929/ETHZ-B-000438728>, 2020.
- Sprenger, M. and Wernli, H.: The LAGRANTO Lagrangian analysis tool - Version 2.0, *Geosci. Model Dev.*, 8, 2569–2586, <https://doi.org/10.5194/gmd-8-2569-2015>, 2015.
- 955 Staley, D. O.: Evaluation of potential-vorticity changes near the tropopause and the related vertical motions, vertical advection of vorticity, and transfer of radioactive debris from stratosphere to troposphere, *J. Atmos. Sci.*, 17, 591 – 620, [https://doi.org/10.1175/1520-0469\(1960\)017<0591:EOPVCN>2.0.CO;2](https://doi.org/10.1175/1520-0469(1960)017<0591:EOPVCN>2.0.CO;2), 1960.
- Stohl, A., Bonasoni, P., Cristofanelli, P., Collins, W., Feichter, J., Frank, A., Forster, C., Gerasopoulos, E., Gäggeler, H., James, P., Kentarchos, T., Kromp-Kolb, H., Krüger, B., Land, C., Meloen, J., Papayannis, A., Priller, A., Seibert, P., Sprenger, M., Roelofs, G. J., Scheel, H. E., Schnabel, C., Siegmund, P., Tobler, L., Trickl, T., Wernli, H., Wirth, V., Zanis, P., and Zerefos, C.: Stratosphere-troposphere exchange: A review, and what we have learned from STACCATO, *J. Geophys. Res.*, 108, 8516, <https://doi.org/10.1029/2002JD002490>, 2003.
- 960 Sutton, R. T., Maclean, H., Swinbank, R., O'Neill, A., and Taylor, F. W.: High-resolution stratospheric tracer fields estimated from satellite observations using Lagrangian trajectory calculations, *J. Atmos. Sci.*, 51, 2995 – 3005, [https://doi.org/10.1175/1520-0469\(1994\)051<2995:HRSTFE>2.0.CO;2](https://doi.org/10.1175/1520-0469(1994)051<2995:HRSTFE>2.0.CO;2), 1994.
- 965 Volonté, A., Joos, H., Lee, M. H. F., Forbes, R. M., and Bouffet-Klein, R.: Identifying the diabatic processes driving the evolution of a sting jet: The case of Storm Ciarán, *EGUsphere* [preprint], pp. 1–36, <https://doi.org/10.5194/egusphere-2025-5225>, 2025.
- Wernli, H. and Davies, H. C.: A Lagrangian-based analysis of extratropical cyclones. I: The method and some applications, *Quart. J. Roy. Meteor. Soc.*, 123, 467–489, <https://doi.org/10.1002/qj.49712353811>, 1997.
- Wernli, H. and Gray, S. L.: The importance of diabatic processes for the dynamics of synoptic-scale extratropical weather systems – a review, *Weather Clim. Dynam.*, 5, 1299–1408, <https://doi.org/10.5194/WCD-5-1299-2024>, 2024.
- 970