Quantifying Isentropic Transport and Mixing in a Modified Lagrangian Coordinate: Applications to Rossby Wave Breaking

Chengji Liu* and Elizabeth A. Barnes

Department of Atmospheric Sciences, Colorado State University, Fort Collins, Colorado

*Corresponding author address: Department of Atmospheric Sciences, Colorado State University, Fort Collins, Colorado.

E-mail: cjliu@atmos.colostate.edu
ABSTRACT

Isentropic transport and mixing are important processes for the distribution of chemical constituents in the mid-to-high latitudes. A new framework is introduced to quantify both isentropic transport and isentropic mixing in a modified Lagrangian coordinate. The framework is applied to quantify the transport and mixing associated with the two types of Rossby wave breaking (i.e. cyclonic and anticyclonic) in two sets of idealized numerical simulations – eddy lifecycle simulations and a long climate simulation. In both sets of simulations, cyclonic wave breaking (CWB) exhibits either comparable or stronger transport and mixing than anticyclonic wave breaking (AWB). Since CWB occurs less frequently when the jet shifts poleward while AWB occurs more frequently, this asymmetry in the transport/mixing associated with the two types of Rossby wave breaking translates into a change in total isentropic transport/mixing when the jet shifts. Specifically, it is found in the climate simulation that as the jet shifts poleward, isentropic eddy mixing (quantified by eddy diffusivity) decreases in the underworld and both eddy mixing and transport across the tropopause decrease in the mid-to-high latitudes. The dynamical relationship above is relevant not only for internal climate variability such as the El-Niño Southern Oscillation (ENSO) and the annular modes, but also, for future climate change that may drive changes in the jet position.
1. Introduction

Atmospheric transport and mixing play a fundamental role in the global distribution of chemical pollutants and moisture. In the extratropics, transport and mixing by eddies is known to mainly operate along isentropic surfaces, i.e. constant potential temperature ($\theta$) surfaces. Within the troposphere, warm conveyor belts embedded in extratropical cyclones transport warm moist air poleward and upward along sloped isentropes (e.g. Thorncroft et al., 1993; Madonna et al., 2014). These transport events are responsible for poleward moisture transport (e.g. Eckhardt et al., 2004) and pollutant transport into the Arctic (e.g. Raatz and Shaw, 1984; Barrie, 1986). In the upper troposphere, vigorous exchange between stratospheric and tropospheric constituents occurs along isentropes across a folding tropopause (e.g. Shapiro, 1980). Such exchange is a major source of ozone in the troposphere (e.g. Lelieveld and Dentener, 2000) where it is considered a pollutant and is detrimental to human health (e.g. Lippmann, 1989). This exchange also injects anthropogenic trace species such as chlorofluorocarbon (CFC) into the stratosphere (Holton et al., 1995).

Due to the dominance of isentropic transport and mixing in the extratropics, $\theta$ is often used as the vertical coordinate in quantifying these processes. Under the adiabatic approximation, $\theta$ can be considered a material surface and hence a Lagrangian coordinate. A Lagrangian coordinate is a more natural choice than an Eulerian one for transport and mixing since it avoids the need for Stokes correction for artifacts arising from the Eulerian-mean (McIntyre, 1980). With $\theta$ being the vertical coordinate, reversible vertical oscillations are absent and any vertical flux is associated with diabatic heating. Along these same lines, it is natural to also choose a conserved variable as the meridional coordinate so that this coordinate is also a material surface in the absence of non-conservative processes such as horizontal diffusion. Examples include using potential vorticity (PV), or the concentration of a passive tracer, as the meridional coordinate (e.g. Butchart and
Remsberg, 1986). By averaging mass with respect to PV or passive tracer contours, a general description of the Lagrangian transport is possible without expensive trajectory calculations.

Conceptually, transport and mixing of a tracer are two different, although related, processes. Their difference lies in the direction of the tracer flux – the direction of transport is dictated by the net mass flux whereas the direction of mixing is determined by the tracer gradient. However, we are not aware of any study that has quantified both processes in a modified Lagrangian coordinate. Nakamura (1995) proposed the modified Lagrangian-mean (MLM) continuity equation to quantify net mass flux both meridionally and vertically, which specifically isolates transport processes. More recent studies that use this framework (e.g. Nakamura, 2007; Yang et al., 2016) are also focused on mass transport alone. On the other hand, Nakamura (1996) studied the distribution of a passive tracer in non-divergent barotropic flow and used the mass (i.e. area) enclosed by the tracer as the meridional coordinate. In such a coordinate, the net mass flux is zero by construction and mixing alone determines the distribution of the passive tracer. Under these conditions, he derived the MLM tracer equation in a diffusive form and proposed the “effective diffusivity”. Other studies that have used the effective diffusivity (or its generalized form) also focus on mixing (e.g. Haynes and Shuckburgh, 2000a,b; Chen and Plumb, 2014; Yang et al., 2014; Abalos et al., 2016). In this study, we propose a new framework to quantify both mass transport (referred to as “transport”) and mixing in a modified Lagrangian coordinate in various synoptic and climate scenarios.

As there are many ways to quantify isentropic transport and mixing, there are many physical processes that drive them. Among the processes that drive isentropic transport and mixing, Rossby wave breaking (RWB) is an important one both within the troposphere and across the tropopause. Near the tropopause, RWB has been shown by numerous studies to be associated with the exchange of mass or chemical tracers between the stratosphere and the troposphere (e.g. Appenzeller and Davies, 1992; Trepte et al., 1993; Chen, 1995; Appenzeller et al., 1996; Jing et al.,
Especially strong exchange occurs in the presence of a double tropopause (e.g. Randel et al., 2007; Pan et al., 2009) which is also a feature related to RWB (e.g. Wang and Polvani, 2011). In the troposphere, RWB has also been linked to the transient transport of moisture (e.g. Ryoo et al., 2013; Payne and Magnusdottir, 2014; Liu and Barnes, 2015).

RWB can be classified into two distinct types – anticyclonic wave breaking (AWB) and cyclonic wave breaking (CWB), and the frequency of each is strongly coupled to the midlatitude jet stream. Climatologically, AWB occurs most frequently on the equatorward flank of the jet where the horizontal wind shear is anticyclonic, while CWB occurs most frequently on the poleward flank of the jet. As the jet shifts poleward, the total frequency of AWB increases whereas that of CWB decreases (e.g. Strong and Magnusdottir, 2008; Woollings et al., 2008; Rivière, 2011; Barnes and Hartmann, 2012). This RWB-jet position relationship is especially important because the jet stream position is very responsive to both internal climate variability such as the El-Niño Southern Oscillation (ENSO) (e.g. Rasmusson and Wallace, 1983; Chen and van den Dool, 1999; Ren et al., 2008), and external climate forcings such as increasing greenhouse gas concentrations and ozone depletion (e.g. Thompson and Solomon, 2002; Butler et al., 2010; Barnes and Polvani, 2013). It is through such coupling that RWB is linked to climate variability on different time scales, and thus can drive the variability of global transport and mixing of various chemical tracers.

Quantifying the transport and mixing by RWB is thus key to understanding the variability of the climate-scale distribution of various chemical tracers. Polvani and Esler (2007) (hereafter PE07) quantified the combined transport and mixing associated with the two types of RWB in idealized eddy lifecycle simulations. They found that CWB exhibits stronger combined transport and mixing from the stratosphere to the troposphere compared to AWB. Considering the coupling of the jet stream position and AWB vs. CWB frequency, such an asymmetry has significant implications since it may translate into a change in total transport and mixing when the jet stream shifts. In
this work, we explore these implications by asking two questions: (1) Is there a robust difference in transport and mixing efficiencies between AWB and CWB? (2) How does this difference, if it exists, translate into a dependence of total transport and mixing on the jet variability?

The paper is organized as follows. A description of the numerical simulations is given in section 2. In section 3, we introduce a new framework to quantify both transport and mixing in a modified Lagrangian coordinate. Section 4 revisits the idealized simulations of PE07 and demonstrates how our new framework can provide additional insight. Section 5 explores the transport and mixing linked to RWB in a climate simulation, and tests the robustness of the asymmetry between AWB and CWB. Section 6 shows how such asymmetry can impact total transport and mixing as the jet-stream shifts. Conclusions are given in section 7.

2. Model setups

All simulations in this study are performed by integrating a primitive equation model with no topography. The specific model used is the Geophysical Fluid Dynamics Laboratory (GFDL) spectral dry dynamical core with a horizontal resolution of T42, and an integrating time step of 1200 seconds. The model use $\nabla^8$ horizontal hyperdiffusion for dynamical variables such as temperature, vorticity and divergence. There is no vertical diffusion for any variable in this model.

With the same model setup described above, we carry out two different sets of simulations. The first set of simulations are idealized eddy lifecycle simulations with initialized passive tracers that follow PE07 (to be discussed in detail). In this simulation, we aim to validate our new framework for quantifying transport and mixing by applying it to stratosphere-troposphere-exchange (STE) in the identical setting used by PE07, and to gain additional insight. The second simulation is an idealized climate run based on Held and Suarez (1994). In this simulation we investigate the asymmetry in RWB-related transport and mixing in an idealized climate setting, and use the
results to explain the dependence of isentropic transport and mixing on jet variability. The detailed configuration for these two simulations is described in the next two subsections.

a. Idealized eddy lifecycle simulation

Following PE07, we reproduce the two idealized eddy lifecycles (LC1 and LC2) first introduced by Thorncroft et al. (1993). The model is configured with 30 unevenly spaced vertical layers and no diabatic heating during the 20-day run. In both the LC1 and LC2 simulations, only the initial conditions are prescribed. For LC1, a baroclinically unstable jet is prescribed on day 1 and the eddies grow and break anticyclonically at the late stages of its lifecycle, which corresponds to AWB in the real atmosphere. The initial zonal wind is given by:

\[ u_1(\phi, z) = U_0 F(\phi) \left[ \frac{z}{z_T} \right] e^{-[(z/z_T)^2-1]/2} \] (1a)

\[ F(\phi) = \begin{cases} \sin(\pi(\sin\phi)^2)^3, & \text{for } \phi > 0 \\ 0, & \text{for } \phi < 0. \end{cases} \] (1b)

where \( z \equiv H \log(p_0/p) \) is the log-pressure height. For LC2, the initial zonal wind is obtained by adding a bottom-heavy cyclonic shear \( u_s \) to the initial wind profile for LC1,

\[ u_2(\phi, z) = u_1(\phi, z) + u_s(\phi, z) \] (2a)

\[ u_s(\phi, z) = -U_s e^{-z/z_s} \left[ \sin(2\phi) \right] \left[ \frac{\phi - \phi_s}{\Delta_s} \right] \left[ \frac{\phi - \phi_s}{\Delta_s} \right] e^{-[(\phi - \phi_s)/\Delta_s]^2} \] (2b)

In the LC2 simulation the eddies grow and break cyclonically at the late stages of the lifecycle which corresponds to CWB. The constants appearing in (1) and (2) are the same as those in PE07. For both lifecycles, the initial conditions for temperature and surface pressure are set to be in thermal wind balance with the zonal wind profiles prescribed in (1) and (2). See appendix A of
PE07 for the additional details on calculating these balanced initial conditions. In addition to the balanced temperature profile, a wavenumber-6 perturbation centered at 45°N is added to the initial temperature field to give rise to the growing eddies.

For both the LC1 and LC2 simulations, the tracer setup is similar to PE07 in that we initialize two passive isentropic tracers: a stratospheric tracer (S) and a tropospheric tracer (T) on isentropes ranging from 290K to 380K. The initial tropopause is defined in PE07 as a nearly vertical boundary that partitions isentropes into a poleward half (stratosphere) and an equatorward half (troposphere) (see Fig. 5 in PE07). The initial concentrations of the two tracers are set such that poleward of the initial tropopause $S = 1$ and $T = 0$, while equatorward of it $T = 1$ and $S = 0$. Since the simulations are adiabatic, $S + T = 1$ on isentropes from 290K to 380K at all times by construction. During the simulations, the tropopause is defined by an evolving boundary between the two tracers as the contour of $S = T = 0.5$. Both $S$ and $T$ are spectral tracers and a $\nabla^8$ hyperdiffusion is applied at each time step. We refer readers to PE07 for additional details.

### b. Idealized climate simulation

We perform a climate simulation forced by the idealized diabatic heating scheme proposed by Held and Suarez (1994). Specifically, we set the diabatic heating as a relaxation to a prescribed zonally-symmetric equilibrium temperature profile:

$$T_{eq} = \max \left\{ 200K, \left[ 315K - (\Delta T)_y \sin^2 \phi - (\Delta \theta)_z \log \left( \frac{p}{p_0} \right) \cos^2 \phi - \epsilon \sin \phi \right] \left( \frac{p}{p_0} \right)^\kappa \right\}$$  \hspace{1cm} (3)

For this relaxation scheme, this is equivalent to a constant heating or cooling term. Idealized as it is, (3) includes the most essential elements of climate forcing – heating in low latitudes and cooling in high latitudes, as represented by term A. Term B is a modification for the tropics, as manifested by the $\cos^2 \phi$ factor. Without term B, but with the inclusion of the factor D, (3) would yield an...
atmosphere that was stratified dry adiabatically. Term B thus can be thought of as a representation of stabilization by moist convection in the tropics which is not represented explicitly in this model setup. Term C adds a hemispheric asymmetry to the equilibrium temperature that accounts for seasonality in radiative forcing. In this study we set $\varepsilon = 10$ which represents winter conditions in the Northern Hemisphere. We focus on winter because the eddy activity is strongest in winter when the baroclinicity is largest. In addition, the low frequency variability that modulates eddy activity (e.g. the annular mode) is also strongest in the winter.

While the equilibrium temperature profile given in (3) leads to a midlatitude circulation that is generally representative of what is observed, there are still noticeable differences, especially in the tropics. For example, the Hadley cell in this dry general circulation model (GCM) is substantially weaker than in observations. However, the main purpose of this simulation is not to reproduce the observed circulation exactly (there is no topography, for example), but to serve as a stepping stone between the unforced eddy lifecycle simulation and reality by removing the complexities of full GCMs that are not essential for isentropic transport and mixing.

To study the transport and mixing along isentropes, we initialize a spectral tracer that has a source in the boundary layer from $60^\circ$S to $60^\circ$N and a sink that includes the entire atmospheric column at the poles so that an equator-to-pole gradient in tracer concentration is maintained along isentropic surfaces. The tracer is otherwise passive throughout the rest of the atmosphere. As will be explained in the next section, this monotonic meridional gradient of the tracer is required for our tracer coordinate system. As in the lifecycle simulations, a $\nabla^8$ hyperdiffusion is used for the tracer.

With the setup described above, the model is run with 20 evenly spaced sigma levels for 25 years. We use the last 22 years for analysis which allows for a spin-up period of about 1000 days. All of the variables are output every 6 hours.
3. Quantification and separation of isentropic transport and mixing

a. MLM framework and the tracer equation

Viewed in an Eulerian framework, the distribution of a passive tracer can be accounted for by two processes: advective fluxes and diffusive fluxes. The idea of MLM is to reformulate the Eulerian tracer equation in a flow-following two-dimensional coordinate so that the advective fluxes are absent. Specifically, we can choose potential temperature ($\theta$) as the vertical coordinate, and the concentration of a passive tracer ($q$) as the meridional coordinate. As shown by Nakamura (1995), under such a coordinate transformation, the mass continuity equation becomes:

$$\frac{\partial \mathcal{M}(1)}{\partial t} = -\frac{\partial \mathcal{M}(\dot{q})}{\partial q} - \frac{\partial \mathcal{M}(\dot{\theta})}{\partial \theta}$$  \hspace{1cm} (4)

where $\dot{q}$ and $\dot{\theta}$ are the material derivatives of $q$ and $\theta$, and

$$\mathcal{M}(\cdot) \equiv \iint_{q^* \leq q} \sigma dA = \int_{q^* \leq q} dq^* \oint_{q^*} \frac{(\cdot)\sigma}{|\nabla_{\theta} q^*|} dl$$  \hspace{1cm} (5a)

$$\frac{\partial \mathcal{M}(\cdot)}{\partial q} = \oint_{q} \frac{(\cdot)\sigma}{|\nabla_{\theta} q^*|} dl$$  \hspace{1cm} (5b)

in which $\sigma \equiv -g^{-1} \frac{\partial p}{\partial \theta}$ is the pseudo-density in isentropic coordinates. Note that in the climate simulation $q$ decreases with latitude as determined by the sources and sinks of our passive tracer.

On the lhs of (4) is the mass tendency within a contour of $q$. The first term on the rhs of (4) accounts for horizontal transport of mass across a contour of $q$, while the second term represents the differential vertical transport of mass across isentropic surfaces. These transport terms are proportional to the magnitudes of $\dot{q}$ and $\dot{\theta}$ which represent non-conservative processes such as diffusion and diabatic heating. These non-conservative processes correspond to irreversible transport and mixing of an air mass. The conservative processes, or in other words, reversible changes due to advection, are invisible to (4).
We can now write the MLM equation for the concentration of a tracer $\chi$:

$$\frac{\partial \mathcal{M}(\chi)}{\partial t} = -\frac{\partial \mathcal{M}(\dot{q}\chi)}{\partial q} - \frac{\partial \mathcal{M}(\dot{\theta}\chi)}{\partial \theta} + \mathcal{M}(\dot{\chi})$$

(6)

and we refer the reader to Appendix A for the derivation. The first three terms are very similar to the three terms in (4). This connection is clearer if one thinks of $\chi$ as a ubiquitous tracer with a concentration of 100% ($\chi=1$) everywhere. In this special case, plugging $\chi=1$ into (6) reduces the tracer equation to the continuity equation (4), where $\mathcal{M}(\dot{\chi})$ vanishes since there are no variations in $\chi$. For a general tracer $\chi$, the first two terms on the rhs of (6) are mass flux weighted by tracer concentration and represent the transport of $\chi$.

The physical meaning of $\mathcal{M}(\dot{\chi})$ is two-folded since $\dot{\chi}$ can be partitioned into two parts:

$$\dot{\chi} = \dot{\chi}_{\text{diff}} + \dot{\chi}_{\text{prod}}$$

The first term is the part due to diffusion ($\dot{\chi}_{\text{diff}}$), and the second term is the part related to tracer production and loss ($\dot{\chi}_{\text{prod}}$), for example, due to chemical reaction or phase change. Due to the linearity of operator $\mathcal{M}(\ )$, we can partition $\mathcal{M}(\dot{\chi})$ accordingly:

$$\mathcal{M}(\dot{\chi}) = \mathcal{M}(\dot{\chi}_{\text{diff}}) + \mathcal{M}(\dot{\chi}_{\text{prod}})$$

(7)

The physical meaning of $\mathcal{M}(\dot{\chi}_{\text{prod}})$ is thus the change in the tracer mass of $\chi$ within a tracer contour of $q$ due to the area-integrated production within the $q$ contour. The reason the production does not show up in (4) is simply that mass cannot be generated or destroyed. In this study, we focus on the dynamic aspect of equation (6) and thus will only use a passive tracer so that $\mathcal{M}(\dot{\chi}_{\text{prod}}) = 0$ at all times. The physical meaning of $\mathcal{M}(\dot{\chi}_{\text{diff}})$ is less straightforward and represents the mixing of tracer $\chi$ into a $q$ contour that is not directly linked to the net mass flux across the contour. The reason this term does not appear in the mass continuity equation (4) is that mixing only swaps mass across the contour. That is, although the air is refreshed on both sides, the
amount of mass on either side remains constant, and thus, total mass flux is zero. We will further justify the interpretation of this term as isentropic mixing in the following subsection.

b. Separation of isentropic transport and mixing

The separation of transport and mixing along isentropes is most clear if we let \( \chi = q \), namely, we use the tracer of interest as our meridional coordinate. In this case, the tracer equation (6) becomes:

\[
\frac{\partial \mathcal{M}(q)}{\partial t} = -\frac{\partial \mathcal{M}(\dot{q})}{\partial q} q - \frac{\partial \mathcal{M}(\dot{\theta}q)}{\partial \theta} + \mathcal{M}(\dot{q}) \tag{8}
\]

where we have used the fact that:

\[
\frac{\partial \mathcal{M}(\dot{q}q)}{\partial q} = \oint_q \dot{q}^* q^* |\nabla \theta q^*| \sigma \, dl = \oint_q \frac{\dot{q}^*}{|\nabla \theta q^*|} \sigma \cdot q = \frac{\partial \mathcal{M}(\dot{q})}{\partial q} q
\]

The first term on the rhs of (8) is simply the meridional net mass flux as shown in (4) times the tracer concentration \( q \). The sign of this term is only determined by the direction of net mass flux and its magnitude is proportional to both the strength of the mass flux and the concentration of the tracer. In light of this, we argue that this term represents the transport of tracer \( q \).

The last term on the rhs of (8) appears as an area integral but can be thought of as a line integral if \( \dot{q} \) takes a diffusive form such as:

\[
\dot{q} = \kappa \nabla^2 q = \kappa \nabla \theta \cdot \nabla q \tag{9}
\]

Plugging (9) into the term \( \mathcal{M}(\dot{q}) \) and applying the divergence theorem leads to

\[
\mathcal{M}(\dot{q}) = \kappa \oint_q |\nabla q^*| \sigma \, dl \tag{10}
\]

The magnitude of \( \mathcal{M}(\dot{q}) \) is thus proportional to the gradient of the tracer \( q \) across the contour.
In the case of non-divergent barotropic flow, $\sigma$ is a constant ($\sigma = \sigma_0$) and we can rewrite $\mathcal{M}(\dot{q})$ in a diffusive form through application of (5b):

$$\mathcal{M}(\dot{q}) = \sigma_0 \kappa_{eff} \frac{\partial q}{\partial A}$$

(11)

where $A(q, \theta, t)$ is the area enclosed by a contour $q$, and

$$\kappa_{eff} = \kappa \frac{\partial}{\partial A} \iint |\nabla \theta q|^2 dA / (\frac{\partial q}{\partial A})^2$$

(12)

is identical to the effective diffusivity proposed by Nakamura (1996). (See Appendix B for the derivation.) The fact that we can write $\mathcal{M}(\dot{q})$ as an effective diffusivity times the tracer gradient further justifies our interpretation of this term as representing mixing. Note that the effective diffusivity $\kappa_{eff}$ in the form of (12) is positive definite so the sign of the mixing is determined only by the tracer gradient in this instance. A previous study (Yang et al., 2016) interpreted the $\mathcal{M}(\dot{q})$ term as representing chemical production only, but as supported above, we argue that this term also includes mixing.

c. Calculation of transport and mixing

To quantify isentropic transport and mixing, we need to calculate the transport and mixing terms in (8). To do this, we need to first determine the tracer contours to use as coordinates. In the idealized lifecycle simulations, the only contour used is the 0.5 contour for both the $S$ and $T$ tracers which defines the tropopause. For the climate simulation, we pick 32 contours of $q$ for each isentropic level in the Northern Hemisphere. What follows describes how these 32 contours are chosen. We determine these 32 values of $q$ by the one-to-one relationship between $q$ and equivalent latitude $\phi_e$ (Butchart and Remsberg, 1986) on each isentrope and at each time step:

$$\phi_e(q) = \arcsin \left[ 1 - \frac{A(q)}{2\pi a^2} \right]$$

(13)
Specifically, we pick 32 values of $\phi_e$ and then obtain the 32 values of $q(\phi_e)$ by reversing the relationship of (13) at each time step. Finally, we temporally average $q(\phi_e)$ over a year of simulation and use these averaged $q(\phi_e)$ as the meridional coordinate. All of the MLM transport and mixing results, however, are displayed with the corresponding equivalent latitude ($\phi_e$) along the x-axis.

The terms in (8) are calculated as area integrals of combinations of $\sigma$ and $\dot{q}$. $\dot{q}$ is calculated as the 4th order hyperdiffusion in the model, and we output $\dot{q}$ at 6-hourly intervals and interpolate it and $\sigma$ on isentropic surfaces following the interpolation scheme of Edouard et al. (1997). The integration area for the numerator of the mass flux term $\partial M(\dot{q})$ is shown in Fig. 1a as a thin green band. The denominator $\partial q$ is calculated as the difference $q_1 - q_2$ of the two contours that bound the green area. The integration area for the mixing term $M(\dot{q})$ is illustrated in Fig. 1b. For the climate simulation, we are especially interested in mixing driven by eddies. To serve this purpose, we partition the integration for $M(\dot{q})$ into two parts following the idea of Chen and Plumb (2014):

$$M(\dot{q}) = \overline{M}(\dot{q}) + \Delta M(\dot{q})$$ (14)

The first term is $\overline{M}(\dot{q})$ which represents the integration poleward of an equivalent latitude circle ($\phi_e$). The integration area for this term is indicated by the black dashed circle in Figs. 1b-d. This term is driven only by diffusion. The second term is $\Delta M(\dot{q})$ which is driven by zonal asymmetries in the flow (i.e. eddies). The integration area of this term is indicated by the shading in Fig 1d where the red area is weighted by 1 and the blue area is weighted by $-1$. $\Delta M(\dot{q})$ captures mixing by eddies (from now on referred to as eddy mixing) and is the component we focus on here.

Although in this study we focus on idealized settings where only passive tracers are used, (8) can be readily applied to more realistic and sophisticated tracers in GCMs in which there is production/loss. In that case, using (8) along with (7) one can separate the contributions from transport, mixing and chemical production and loss to the distribution of a species.
d. Linking transport and mixing to Rossby wave breaking

For the idealized lifecycle simulations, linking transport and mixing to the two types of wave breaking is straightforward. As in PE07, we assume all of the transport and mixing in the LC1 simulation is linked to AWB while all of the transport and mixing in the LC2 is linked to CWB. However, for the climate simulation in which AWB and CWB coexist every day along with other non-breaking waves, we need a dedicated algorithm to separate the contribution from the two types of wave breaking from all of the other processes. To serve this purpose, we need to detect the two types of RWB (AWB and CWB) in the model output. Unlike some previous studies where contours of potential vorticity on isentropes are used to identify wave breaking events (e.g. Strong and Magnusdottir, 2008; Liu et al., 2014; Liu and Barnes, 2015), we base our algorithm on the tracer contours themselves. In fact, the contours of the tracer $q$ in our climate simulation align well with PV contours on isentropic surfaces and thus our method is very similar to that of previous studies (not shown). The reason we favor $q$ over PV for RWB detection is that our quantification of the transport and mixing is based on $q$ contours already. Thus, using $q$ to detect RWB is natural for linking transport and mixing to RWB events in our framework.

Specifically, we detect RWB based on the wave lobes illustrated in Figs. 1c and 1d. If the leftmost/rightmost point of one lobe is to the left/right of its base line (shown as black dashed segments), then we identify the lobe as overturning. We require the extent of overturning be at least 5.5° of longitude to exclude small scale disturbances that are not linked to large-scale RWB. Then, according to the direction of overturning, we partition the overturning lobes into AWB and CWB. For example, in Fig. 1d, the overturning lobe is identified as CWB and marked by dark blue shading. The eddy mixing $\Delta \mathcal{M}(q)$ associated with this CWB lobe is the integration over the dark blue area in Fig. 1d. Similarly, the transport associated with the CWB lobe is the part of
the transport integration that overlaps with the lobe, as illustrated by dark green region in Fig. 1c. The frequency of occurrence of RWB is defined as the ratio of RWB area to the total wave area (e.g. dark blue versus all shading in Fig. 1d). We compared the climatology of RWB frequency obtained by this method with that obtained by an algorithm using PV contours (Liu et al., 2014; Liu and Barnes, 2015). They agree well with each other (not shown), thus further supporting our use of $q$ for identifying RWB in this study.

4. Idealized lifecycle simulations

With the new framework to quantify transport and mixing introduced in the last section, we aim to achieve two goals in this section: (1) validate our new framework for quantifying and separating transport and mixing, and (2) gain additional insight into the STE in the idealized experiments explored by PE07.

Figure 2 shows snapshots of tracer $S$ on the 335K isentrope in the two idealized lifecycles, as also shown by PE07. Orange indicates the stratosphere and blue indicates the troposphere. On day 8, the anticyclonic overturning in LC1 is depicted by the blue shading equatorward of the tropopause (denoted by the black dashed line), and the cyclonic overturning in LC2 is depicted by orange shading poleward of the tropopause (Figs. 2c and 2d respectively). It is evident in Figs. 2c and 2d that CWB in LC2 is much more active in stretching and overturning the tropopause compared to AWB in LC1. As a result, there is a larger interface between the $S$ and $T$ tracers for transport and mixing for CWB. Consistent with this picture, PE07 documented 50% stronger stratosphere-to-troposphere transport and mixing in LC2 than in LC1.

Figure 3 shows the detailed quantification of STE in the two idealized lifecycles. Dashed blue lines in the upper row shows the troposphere-to-stratosphere combined transport and mixing quantified using PE07’s method. Specifically, we show the evolution of the mass of tracer $T$ poleward
of the tropopause (0.5 contour) in the LC1 (left) and LC2 (right) simulations. This corresponds to the time integration of the $\frac{\partial M(q)}{\partial t}$ term in (8) poleward of $q = 0.5$, with $q = T$. Positive slopes of the blue lines indicate an increase of $T$ in the stratosphere, or a poleward combined transport and mixing of tracer $T$ into the stratosphere. Similarly, dashed blue lines in the bottom row of Fig. 3 show the stratosphere-to-troposphere combined transport and mixing by integrating the mass of $S$ poleward of the 0.5 contour. Negative slopes of the blue lines indicate a decrease of $S$ in the stratosphere, or an equatorward combined transport and mixing of tracer $S$ into the troposphere. The dashed blue lines in Fig. 3 agree qualitatively with PE07 – LC2 is comparable to LC1 in terms of troposphere-to-stratosphere combined transport and mixing but has much stronger stratosphere-to-troposphere combined transport and mixing compared to LC1.

So far we have only looked at the combined transport and mixing in these lifecycle simulations. With our new framework, we can now quantify transport and mixing separately. Transport is depicted as green lines while mixing is depicted as red lines in Fig. 3. Specifically, what is shown is the time integration of the transport and mixing terms in (8). Since the simulations are adiabatic, the second term on the $rhs$ of (8), which represents the vertical transport by diabatic processes, is zero. This means the sum of the transport and mixing terms should equal the total tracer change, namely, the sum of the green and red lines should align with the dashed blue lines. We verify this by plotting the sum of the transport and mixing as solid blue lines in Fig. 3, and they align well with the dashed blue lines. Note that the dashed and solid blue lines are obtained by totally independent methods, one being the integration of the tracer mass and the other being the integration of the small-scale diffusion of the tracer. Considering this, the fact that they align well with each other lends strong support to our new method for calculating isentropic transport and mixing.
Taking a closer look at the evolution of transport and mixing in Fig. 3, one finds a symmetry between the upper and lower panels. First, the green lines (which indicate transport) are the same between the upper and lower panels. This is because transport is the product of net mass flux and tracer concentration. Since in all cases the transport is evaluated at $S = T = 0.5$, both the net mass flux and the tracer concentration are the same for the two tracers. Secondly, the red lines (which indicate mixing) are in the exact opposite directions for $q = T$ and $q = S$. This is due to the fact that $S = 1 - T$, or in other words, the two tracers constitute the whole air mass. As a result, $S$ and $T$ have gradients of the same magnitude but in opposite directions. Since the mixing is determined by the gradient of the tracer, opposite gradients give rise to opposite mixing. Another feature that stands out in Fig. 3 is that the mixing (red lines) exhibits a monotonic change with time. This is because mixing is usually down-gradient and the gradient of the tracer is fixed to be the same sign by construction throughout the entire simulation. Specifically, the down-gradient direction for tracer $T$ is always poleward and thus the mixing of $T$ is poleward (positive; Figs. 3a and 3b), while the down-gradient direction for tracer $S$ is equatorward and the mixing of $S$ is thus always equatorward (negative; Figs. 3c and 3d).

If we compare the transport and mixing terms for LC1 and LC2 in Fig. 3, we see that LC2 has both stronger transport and stronger mixing compared to LC1, consistent with what one might expect from Fig. 2. In both LC1 and LC2, the direction of mass transport is equatorward from the stratosphere to the troposphere (negative green lines in Figs. 3a-d). For the tropospheric tracer $T$, this means that the direction of transport opposes the direction of mixing (Figs. 3a and 3b). Before day 4, poleward mixing of tracer $T$ into the stratosphere dominates over the transport due to the large initial gradient of $T$. After day 4, the stratosphere has been loaded with some $T$ tracer and the equatorward mass transport starts to bring some of this $T$ tracer back in to the troposphere. As a result, although LC2 exhibits stronger transport and mixing, the net change in mass of $T$
in the stratosphere ends up being similar to that of LC1 (blue lines in Figs. 3a and 3b). For the stratospheric tracer $S$, the directions of transport and mixing are the same (Figs. 3c and 3d). After day 4, as equatorward mixing increases $S$ in the troposphere, the equatorward mass flux also brings even more $S$ tracer from the stratosphere to the troposphere. As a result, LC2 with both stronger transport and mixing exhibits significantly stronger combined transport and mixing compared to LC1.

Section summary

We applied our new framework to quantify MLM transport and mixing in the idealized lifecycle simulations of PE07. The results of this analysis can be summarized by the following two conclusions:

- the new framework is able to close the budget of tracer mass in both LC1 and LC2.
- CWB has both stronger transport and mixing than AWB across an idealized tropopause.

In the next section, we show how the second result (and others) manifest in a full climate simulation.

5. Climatology of transport and mixing

Figure 4 shows the climatology of potential temperature (solid line) in pressure coordinates from the idealized climate simulation. The shading denotes the range of isentropes (270K-350K) on which we quantify transport and mixing of the idealized tracer. We further divide the shaded area into the middleworld (green shading, 300K-350K) and the underworld (pink shading, 270K-295K) (e.g. Shaw and Austin, 1930; Hoskins, 1991). The underworld is defined by isentropes that are always below the tropopause denoted by a black dashed line, while the middleworld is defined...
by isentropes that cross the tropopause. In the rest of the paper, the majority of the results are shown on these isentropes or as an average over the underworld or the middleworld.

As shown by equation (8), both transport and mixing are influenced by the tracer distribution. Since the tracer setup here does not represent any specific chemical tracer in the real atmosphere, it would not be generally relevant to show its transport and mixing. Fortunately, we can readily extract information more applicable to general situations by calculating the net mass flux (rather than tracer mass flux) to quantify transport and calculating eddy diffusivity to quantify mixing. The net mass flux is calculated as $-\frac{\partial \mathcal{M}(\dot{q})}{\partial \dot{q}}$ in the transport term in (4). The eddy diffusivity is calculated as the eddy mixing term $\Delta \mathcal{M}(\dot{q})$ from (14) normalized by the tracer gradient, that is, $\Delta \mathcal{M}(\dot{q}) \frac{a \partial \phi}{\partial q}$. Note that this expression of eddy diffusivity is very similar to that of Chen and Plumb (2014) which employs a hybrid Eulerian-Lagrangian mean coordinate. The difference is that they further factor out the mass making the units the same as small-scale diffusion ($m^2 \cdot s^{-1}$).

In the rest of this paper, only the net mass flux and eddy diffusivity are shown to quantify transport and mixing respectively.

Figure 5a shows the spatial pattern of climatological meridional net mass flux (shading) and the midlatitude jet (black solid contours). The net mass flux is generally poleward in midlatitudes and equatorward at higher latitudes. In the subtropics, between 310K and 320K, there is very intense equatorward mass flux there. Its large magnitude is partly due to the fact that the mass represented by these few isentropes is very large (Fig. 4). Near the tropopause in midlatitudes, the transport does not seem to be affected by the existence of the jet stream, indicating that jet does not act as a barrier to transport. Fig. 5b shows the contribution by RWB to the mass transport (shading) and Figs. 5c and 5d further divides the RWB-related mass transport into AWB and CWB contributions. The total RWB contribution resembles the total transport in most regions. The only exception occurs near the jet core where total transport is poleward while RWB transport is absent. AWB
contributes more at lower latitudes while CWB contributes more at higher latitudes. Poleward of
45°N equivalent latitude across the tropopause, CWB dominates the total RWB transport.

The frequency of total RWB, AWB and CWB are shown as grey solid lines in Fig. 5b-d. In
Fig. 5b, RWB frequency minimizes at the jet core and maximizes on both flanks of the jet and
beneath the jet core. Dividing this frequency into AWB and CWB components, we see AWB
mainly occurs at lower latitudes equatorward of the jet where the mean horizontal wind shear is
anticyclonic (Fig. 5c), while CWB mainly occurs at higher latitudes poleward of the jet where the
mean shear is cyclonic (Fig. 5d). The spatial distribution of AWB and CWB frequencies viewed in
this tracer coordinate exhibit some additional interesting features. Above the troposphere, there is
a clear spatial division between the two types of RWB and they rarely overlap. In the troposphere,
however, they largely overlap in midlatitudes between 40°N and 50°N equivalent latitude. As
will be shown in the next section, such differences give rise to different behavior of RWB-related
transport and mixing in the middleworld and in the underworld with regard to jet stream variability.

The spatial pattern of the climatological eddy diffusivity is shown in Fig. 6a as red shading
along with the jet stream (black solid contour). Unlike for mass transport, mixing does minimize
at the jet core near the tropopause, indicating that the jet acts as a mixing barrier (e.g. Haynes
and Shuckburgh, 2000b; Chen and Plumb, 2014). Such differences in the behaviors of transport
and mixing highlight the necessity to differentiate them. The eddy diffusivity linked to RWB
bears a very similar spatial pattern to the total (Fig. 6b), and in this model about 50% of eddy
mixing is related to large-scale RWB. The RWB frequency of occurrence agrees well with the
magnitude of the eddy diffusivity, with the largest eddy diffusivities overlapping the maxima of
RWB frequencies. The maxima at higher latitudes is associated with CWB while the maxima at
lower latitudes is related to AWB (Figs. 6c and 6d).
A true comparison of the transport and mixing between the two types of RWB can be obtained by dividing their climatological mean values by the frequency of RWB occurrence. Through this normalization, we factor out the contribution of frequency and compare the transport and mixing per occurrence of AWB/CWB, i.e., their efficiencies. In most of the underworld, AWB and CWB transport have the same sign and comparable transport efficiencies (not shown), that is, a single occurrence causes the same mass transport. In the middleworld between $45^\circ N$ and $60^\circ N$, AWB and CWB have opposite signed mass transport. Specifically, AWB transports mass equatorward and CWB transports mass poleward across the tropopause (Figs. 5c and 5d).

Mixing efficiencies for the two types of RWB are shown in Figs. 7c and 7d, along with their counterparts from the idealized eddy lifecycle simulations in Figs. 7a and 7b. In both the lifecycle and climate simulations, CWB (LC2) exhibits a larger diffusivity than AWB (LC1) in the midlatitudes. The difference is especially evident in the climate simulation near $50^\circ N$ equivalent latitude (Figs. 7c and 7d). The lifecycle simulations bear much resemblance to the climate simulations in Fig. 7, indicating the relevance of the idealized lifecycle simulations to more realistic climate settings. Recall that the lifecycle simulations are only made of one event, while the climate simulation is composed of thousands. Thus, we do not expect the results to be identical. However, it is striking that they both agree on the existence of negative diffusivity equatorward of the jet stream in the subtropics, and that this feature is only linked to CWB (Figs. 7b and 7d). Such up-gradient mixing behavior has been documented in reanalysis data within a similar latitude range (Birner et al., 2013), and this result indicates that such behavior might be related to a specific type of wave breaking.
Section summary

We show the climatology of transport and mixing, quantified by net mass flux and eddy diffusivity in a climate simulation and find,

- the jet stream acts as a mixing barrier near the tropopause but not a transport barrier,
- CWB has a comparable net transport efficiency but significantly stronger mixing efficiency than AWB in the underworld.

In the next section, we show how such asymmetry in RWB diffusivity translates into the dependence of mixing on jet variability.

6. Dependence on jet stream variability

The dependence of transport and mixing on the internal variability of the jet, specifically the latitudinal shifts of jet, is explored by compositing the transport and mixing with respect to various jet latitudes. We calculate the jet latitude as the latitude of maximum 850hPa zonal-mean zonal wind at 6-hour resolution (e.g. Barnes and Hartmann, 2010; Woollings et al., 2010). We group the jet latitudes into four bins centered at 39°N, 43°N, 47°N, and 51°N. These latitudes are chosen to make each bin have a similar sample size. We then composite RWB frequency, total transport and mixing, and the contribution by RWB according to these jet latitude bins.

a. Tropospheric transport and mixing

The tropospheric transport and mixing are investigated by focusing on the underworld, which constitutes a corridor between the midlatitude boundary layer and the polar middle-to-upper troposphere (Fig. 4). The average frequency of RWB in this corridor is shown in Fig. 8. Consistent with previous studies, AWB occurs more frequently while CWB occurs less frequently as the jet
moves poleward. The extent of the frequency change associated with AWB and CWB are com-
parable in midlatitudes around 45°N. This indicates the compensation between the two types of
RWB when the jet shifts around, keeping RWB frequency relatively constant in the midlatitudes
(Fig. 8c).

Figure 9 shows the composite mass transport and the contribution from RWB for various jet lat-
itudes. RWB contributes less than 20% of the total mass transport in the subtropics and about 50%
poleward of 55°N equivalent latitude. Neither total transport nor RWB transport show significant
change when the jet wobbles around (Figs. 9a and 9b). At least for the RWB contribution, this is
due to the opposing changes in frequency of AWB and CWB (Figs. 8a and 8b), combined with
the fact that the two types have comparable transport efficiencies in the underworld. As a result,
the change in mass transport associated with AWB and CWB largely cancel each other (Figs. 9c
and 9d) and leave the RWB transport unchanged (Fig. 9b).

Figures 10a and 10b show the total eddy diffusivity and the contribution from RWB. RWB con-
tributes slightly more than half of the total and both the total and RWB-contributions to eddy
diffusivity decrease when the jet is more poleward, in contrast to the case of transport. The dif-
ference lies in the fact that CWB has a significantly stronger eddy diffusivity than AWB (Figs. 7c
and 7d). As a result, the decrease in CWB diffusivity overwhelms the increase in AWB diffusivity
although their changes in frequency of occurrence are comparable (Fig. 8). This effect is most
evident in the midlatitudes around 45°N equivalent latitude. In this case, the asymmetry between
AWB and CWB mixing efficiencies is key to determining the change in total eddy diffusivity
linked with changes in the jet position.
b. Stratosphere-troposphere exchange (STE)

As shown in Fig. 2, RWB promotes STE by distorting the tropopause. The vertical distortion of the tropopause by AWB and CWB in the idealized lifecycle simulations is demonstrated in Fig. 11 by snapshots on day 6 and day 7 respectively. The two dates are chosen for the peak stage of AWB and CWB transport/mixing (Fig. 3). In Fig. 11, both AWB and CWB are associated with an intrusion of stratospheric air that extends as low as 850hPa. These streamers are also observed in nature (e.g. Shapiro, 1980) and are responsible for injecting anthropogenic pollutants into the stratosphere and bringing ozone-rich stratospheric air down to the boundary layer. Quantifying the variability of RWB-related STE as shown in Fig. 11 is hence of great interest. To serve this purpose, the tropopause is defined as the mean 2PVU surface for the four jet latitudes, and composite transport and mixing are correspondingly extracted along the tropopauses for the four jet latitudes.

The composite frequencies of occurrence of the two types of RWB in the middleworld are shown in Fig. 12 with respect to jet latitude. AWB mainly occurs equatorward of the jet while CWB mainly occurs poleward of the jet and there is little overlap. When the jet shifts poleward, AWB occurs more frequently while CWB occurs less frequently. Figures 13a and 13b show the total mass transport across the tropopause and the contribution from RWB. Both the total and RWB contribution exhibit troposphere-to-stratosphere transport equatorward of 55°N equivalent latitude and stratosphere-to-troposphere transport poleward of 55°N. In terms of the variability associated with the jet shifting, a substantial portion of the total can be explained by the RWB contribution (compare Figs. 13a and 13b), which in turn, is dominated by CWB (Fig. 13c). Such dominance is largely due to the stronger decrease in CWB frequency compared to the increase in AWB frequency (Fig. 12). As such, the total transport across the tropopause shifts poleward and weakens
as the jet shifts poleward. Due to the same line of reasoning, the variability of eddy diffusivity along the tropopause is also dominated by the changes in CWB frequency, with the maximum diffusivity shifting poleward and weakening as the jet shifts poleward (Fig. 14).

c. Section summary

As the jet shifts poleward,

- underworld transport does not change due to the compensating frequency changes of AWB and CWB, and their similar transport efficiencies.

- underworld eddy diffusivity decreases due to the asymmetry in AWB and CWB mixing efficiencies.

- across the tropopause, both mass transport and mixing decrease due to the dominating decrease in CWB frequency.

7. Conclusions

A new framework to quantify separately both isentropic transport and mixing is proposed and applied to Rossby wave breaking (RWB) in both free eddy lifecycle simulations and a forced climate simulation. The focus of this study is on the asymmetry between the two flavors of RWB – anticyclonic wave breaking (AWB) and cyclonic wave breaking (CWB). It is found that in both sets of simulations and throughout different regions of the atmosphere, CWB has either comparable or stronger isentropic transport and mixing than AWB. This result has implications for the influence of climate variability on transport and mixing. Since CWB occurs less frequently and AWB occurs more frequently as the jet shifts poleward, such asymmetry translates into a decrease in mixing
strength (eddy diffusivity) within the troposphere, and decrease in both transport and mixing across the tropopause, as the jet shifts poleward.

Although the simulations in this study are highly idealized, we argue that the conclusions obtained are applicable to the real atmosphere. Abalos et al. (2016) used ERA-Interim to show that in winter the effective diffusivity across the tropopause decreases in the mid-to-high latitudes during a positive Northern Annular Mode when the jet is more poleward, and increases during positive ENSO when the jet is more equatorward. These results are consistent with the modulation of the jet stream on the two types of RWB. Although our study does not directly address the jet shift in response to external forcing (e.g. anthropogenic climate change), we expect similar results to what is found here due to the same relationship between RWB and the jet stream in climate change simulations (e.g. Barnes and Polvani, 2013). In fact, Orbe et al. (2015) demonstrated that transport and mixing from the midlatitude boundary layer to the Arctic increases over the northeast Pacific with climate change in a state-of-the-art GCM where the jet stream shifts equatorward. This is consistent with our argument that an equatorward jet shift increases the frequency of cyclonic wave breaking, and thus, increases the high-latitude transport and mixing.

In the real atmosphere, certain constituents whose spatial distributions are subject to climate change, also contribute to the climate forcing. Examples include carbon dioxide, ozone, various species of aerosols and water vapor. Understanding the passive response of these atmospheric constituents to climate change is thus an important step towards understanding the entire feedback. This study provides a quantification methodology and a mechanistic explanation for how the transport and mixing of these constituents may respond to future variability and change.

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Derivation of modified Lagrangian mean (MLM) tracer equation

The derivation of the MLM tracer equation is to a large extent a mathematical transformation that starts with:

$$\frac{\partial \mathcal{M}(\chi)}{\partial t} = \frac{\partial}{\partial t} \int \sigma \chi dA - \int \frac{\partial}{\partial \theta} \int \sigma \chi \frac{\partial q^*}{\partial \theta} dA$$  \hspace{1cm} (A1)

The only physics that comes in is that of mass conservation:

$$\frac{\partial (\sigma \chi)}{\partial t} = -\nabla \theta \cdot (\sigma \chi u) - \frac{\partial}{\partial \theta} (\sigma \chi \dot{\theta}) + \sigma \dot{\chi}$$  \hspace{1cm} (A2)

$$\frac{\partial q^*}{\partial t} = -u \cdot \nabla \theta q^* - \dot{\theta} \frac{\partial q^*}{\partial \theta} + \dot{q}^*$$  \hspace{1cm} (A3)

where $\dot{\chi}$ and $\dot{q}^*$ represent non-conservative processes such as diffusion and/or production of the two tracers. Substituting (A2) and (A3) into (A1) and re-arranging,

$$\frac{\partial \mathcal{M}(\chi)}{\partial t} = -\int \nabla \theta \cdot (\sigma \chi u) dA + \frac{\partial}{\partial \theta} \int \sigma \chi u \cdot \nabla \theta q^* dA + \frac{\partial}{\partial \theta} \int \sigma \chi \frac{\partial q^*}{\partial \theta} dA$$

$$- \int \sigma \chi \dot{\theta} dA + \int \sigma \dot{\chi} dA$$  \hspace{1cm} (A4)

Applying the divergence theorem to the first term on the rhs of (A4) and using the relation (5b) leads to:

$$-\int \nabla \theta \cdot (\sigma \chi u) dA = -\int q \sigma \chi u \cdot \frac{\nabla \theta q^*}{|\nabla \theta q^*|} dl = -\frac{\partial}{\partial q^*} \int \sigma \chi u \cdot \nabla \theta q dA$$  \hspace{1cm} (A5)

Substituting (A5) into (A4) and noting that:

$$\frac{\partial}{\partial q^*} \int \sigma \chi \frac{\partial q^*}{\partial \theta} dA - \int \frac{\partial (\sigma \chi \dot{\theta})}{\partial \theta} dA = -\frac{\partial}{\partial \theta} \int \sigma \chi \dot{\theta} dA$$  \hspace{1cm} (A6)

one obtains:

$$\frac{\partial \mathcal{M}(\chi)}{\partial t} = -\frac{\partial}{\partial q^*} \int \sigma \chi q^* dA - \frac{\partial}{\partial \theta} \int \sigma \chi \theta dA + \int \sigma \dot{\chi} dA$$

$$= -\frac{\partial \mathcal{M}(\dot{q} \chi)}{\partial q} - \frac{\partial \mathcal{M}(\dot{\theta} \chi)}{\partial \theta} + \mathcal{M}(\dot{\chi})$$  \hspace{1cm} (A7)
APPENDIX B

Derivation of effective diffusivity

Instead of assuming (9), we assume a more general form of hyperdiffusion for 2-D flow:

\[
\dot{q} = \kappa \nabla^{2m} q = \kappa \nabla \cdot \nabla^{2(m-1)} q
\]  
(B1)

where (9) is the special case in which \( m = 1 \). Plugging (B1) into \( \mathcal{M}(\dot{q}) \) leads to:

\[
\mathcal{M}(\dot{q}) = \sigma_0 \kappa \int \nabla \cdot \nabla^{2(m-1)} q^* \, dA
\]

Using the divergence theorem,

\[
\mathcal{M}(\dot{q}) = \sigma_0 \kappa \int q^* \nabla^{2(m-1)} q^* \cdot \nabla q^* / |\nabla q^*| \, dl
\]

and using relation (5b):

\[
\mathcal{M}(\dot{q}) = \sigma_0 \kappa \frac{\partial}{\partial q} \int \nabla^{2(m-1)} q^* \cdot \nabla q^* \, dl
\]

\[
= \sigma_0 \kappa \frac{\partial}{\partial A} \int \nabla^{2(m-1)} q^* \cdot \nabla q^* \, dl \frac{\partial A}{\partial q} \frac{\partial q}{\partial A} \left( \frac{\partial q}{\partial A} \right)^2 \kappa_{eff}
\]  
(B2)

This form of effective diffusivity \( \kappa_{eff} \) is identical to that in Nakamura and Zhu (2010) (appendix D). Letting \( m = 1 \), \( \kappa_{eff} \) takes the form of (12) which is identical to that in Nakamura (1996).

Note that we could use (B2) to calculate the mixing term \( \mathcal{M}(\dot{q}) \) since in our model \( \dot{q} \) does take a hyperdiffusion form. However, we choose to directly integrate the small-scale diffusion \( \dot{q} \) to be consistent with our calculation of the transport term \(- \partial \mathcal{M}(\dot{q})/\partial q\).
References


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\[
\mathcal{M}(q)\bigg|_{t_0}^t = -\int_{t_0}^t q \frac{\partial \mathcal{M}(\dot{q})}{\partial q} dt + \int_{t_0}^t \mathcal{M}(\dot{q}) dt
\]

**FIG. 3:** Time integration of transport (green) and mixing (red) of tracer \( T \) and \( S \) for LC1 and LC2 simulations (unit: \( 1 \times 10^{16} \) kg). Dashed blue lines denote the actual change in tracer mass due to transport and mixing, with the solid blue lines denoting that estimated by the sum of the transport and mixing terms (solid blue = solid red + solid green). Positive (negative) values denote a poleward (equatorward) transport/mixing into the stratosphere (troposphere).
Fig. 4: Climatology of zonal-mean potential temperature $\theta$ in the 25-year climate run (solid contours, unit: K). The dashed line denotes the climatological 2 PVU surface which represents the dynamical tropopause. Pink and light green shading denote the underworld and the middleworld analyzed here.
Fig. 5: Climatology of mass transport (shading) for the (a) total, (b) Rossby wave breaking (RWB) contribution, (c) anticyclonic wave breaking (AWB) contribution, and (d) cyclonic wave breaking (CWB) contribution. The two solid black contours in (a) denote the 20 m/s and 30 m/s contours of the zonal mean zonal wind. Contours in (b)-(d) denote the frequency of occurrence of (b) RWB, (c) AWB, and (d) CWB events, with a contour interval of 0.15. The black dashed line is the 2PVU contour that represents the dynamical tropopause.
Fig. 6: Climatology of eddy diffusivity (shading) for the (a) total, (b) Rossby wave breaking (RWB) contribution, (c) anticyclonic wave breaking (AWB) contribution, and (d) cyclonic wave breaking (CWB) contribution. The two solid black contours in (a) denote the 20 m/s and 30 m/s contours of the zonal mean zonal wind. Contours in (b)-(d) denote the frequency of occurrence of (b) RWB, (c) AWB, and (d) CWB events, with a contour interval of 0.15. The black dashed line is the 2PVU contour that represents the dynamical tropopause.
Fig. 7: (a)-(b): Eddy diffusivity (shading) in the idealized lifecycle simulations averaged over days 5-13 for (a) LC1, and (b) LC2. (c)-(d): Climatology of eddy diffusivity in the 25-year climate simulation for (c) anticyclonic wave breaking (AWB), and (d) cyclonic wave breaking (CWB), normalized by their respective frequency of occurrence.
Fig. 8: Composite frequency of occurrence of Rossby wave breaking (RWB) with respect to various jet positions for (a) anticyclonic wave breaking (AWB), (b) cyclonic wave breaking (CWB), and (c) the total RWB in the underworld (270-295K).
Fig. 9: Composite mass transport (unit: $1 \times 10^{14}$ kg/s) in the underworld with respect to various jet positions for (a) the total, (b) Rossby wave breaking (RWB), (c) anticyclonic wave breaking (AWB), and (d) cyclonic wave breaking (CWB).
Fig. 10: Composite eddy diffusivity (unit: $1 \times 10^{14} \text{kg} \cdot \text{m/s}$) in the underworld with respect to various jet positions for (a) the total, (b) Rossby wave breaking (RWB), (c) anticyclonic wave breaking (AWB), and (d) cyclonic wave breaking (CWB).
Fig. 11: Snapshots of stratospheric tracer concentration (shading) in the (a) LC1, and (b) LC2 idealized lifecycle simulations on the day of maximum intensity. The black dashed line denotes the zonal-mean contour of 2PVU averaged over the eddy life cycle.
Fig. 12: Composite frequency of occurrence of Rossby wave breaking with respect to various jet positions for (a) anticyclonic wave breaking (AWB), and (b) cyclonic wave breaking (CWB) in the middleworld (300-350K).
Fig. 13: Composite mass transport (unit: $1 \times 10^{14} \text{kg/s}$) across the dynamical tropopause with respect to various jet positions for (a) the total, (b) Rossby wave breaking (RWB), (c) anticyclonic wave breaking (AWB), and (d) cyclonic wave breaking (CWB).
FIG. 14: Composite eddy diffusivity (unit: $1 \times 10^{20} \text{kg} \cdot \text{m/s}$) along the dynamical tropopause with respect to various jet positions for (a) the total, (b) Rossby wave breaking (RWB), (c) anticyclonic wave breaking (AWB), and (d) cyclonic wave breaking (CWB).