Regionally Resolved Diagnostic of Transport: A Simplified Forward Model for CO2

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ABSTRACT

Simply diagnostic tools are useful for understanding transport processes in complex chemistry transport models (CTMs). For this purpose, a combined use of the airmass origin fractions (AOFs) and regionally resolved mean ages (RMAs) is presented. This approach merges the concept of the origin of air with the well-known theory of the mean age of air (AoA) for different regions covering the whole Earth. The authors show how the AoA calculated relative to Earth’s surface can be decomposed into regionally resolved components (i.e., into RMAs). Using both AOFs and RMAs, the authors discuss differences in the seasonality of transport from the Northern and Southern Hemispheres into the tropical tropopause layer (TTL), the asymmetries of the interhemispheric exchange, and differences in relation to the continental or oceanic origin of air. Furthermore, a simplified transport model for a chemically passive species (tracer) is formulated that has some potential to approximate the full transport within a CTM. This analytic approach uses the AOFs as well as the RMAs as parameters to propagate a tracer prescribed on Earth’s surface (lower boundary condition). This method is exactly valid for sources that change linearly with time in each of the considered regions. The authors analyze how well this approach approximates the propagation of CO2 from the planetary boundary layer (PBL) into the whole atmosphere. The CO2 values in the PBL are specified by the CarbonTracker dataset. The authors discuss how this approach can be used for inverse modeling of CO2.

1. Introduction

Although tropospheric air enters the stratosphere predominantly through the tropical tropopause layer (TTL) (Fueglistaler et al. 2009), there is a wide range of pathways connecting the planetary boundary layer (PBL) with the TTL itself (e.g., Levine et al. 2007; Randel et al. 2010; Vogel et al. 2011). Different diagnostics have been developed to quantify such pathways. The age spectrum of air has been shown to be a comprehensive diagnostic of atmospheric transport defining the composition of air as a probability density function (PDF) of transit times from a prescribed source region to the considered space–time point (e.g., Hall and Plumb 1994; Waugh and Hall 2002; Orbe et al. 2015, 2016).

In addition to the assumption that chemistry does not affect the transported (idealized) species (i.e., the tracers), the definition of the source region is another limiting factor in determining the age spectrum. Typically, the tropical tropopause is considered as a source region if only stratospheric transport is envisaged. Another useful choice is to consider Earth’s surface, relative to which the PDF of the transit times has to be determined. In such a case, transport within the troposphere can also be diagnosed.

However, it might also be useful to compare transport from different parts of Earth, for example, to contrast the contributions of the oceans relative to the continents or of the northern relative to the Southern Hemisphere (Holzer 2009; Orbe et al. 2015; Tissier and Legras 2016). Furthermore, if emissions such as carbon dioxide (CO2) are considered, it can also be useful to quantify transport from different continents or even countries. Although a regionally resolved diagnostic of transport in terms of age spectra is a natural generalization (Holzer and Boer 2001), its implementation would require large computer resources as the calculation of age spectra for only one source region is a demanding and resource-intensive task (Haine et al. 2008; Ploeger and Birner 2016).

Commonly, only parts of the age spectrum can be derived from measurements, typically those describing the
fast transport to the considered space–time point and, consequently, quantifying the contribution of young air within the age spectrum (Ehhalt et al. 2007). Furthermore, the first moment of the age spectrum [i.e., the mean age of air (AoA) (Hall and Plumb 1994)] can also be derived from the observations and is widely used, for example, to quantify differences in stratospheric transport among comprehensive climate models (Eyring et al. 2010).

Recently, Orbe et al. (2013, 2015) introduced a climatology of mass fractions of air originating from different regions on Earth and entering the stratosphere. As we discuss later, such mass fractions can also be understood as zero moments of the regional age spectra. In addition, Waugh et al. (2013) and Orbe et al. (2016) also discussed the seasonality of the mean age from the Northern Hemisphere (NH), which is an example of the regionally resolved mean age. Following the spirit of these investigations, we divide the whole Earth into different regions and in this paper analyze how transport can be diagnosed in terms of the airmass origin fractions (AOFs) and the regionally resolved mean ages (RMAs).

First, we investigate the differences in the seasonality of the air composition in the TTL with respect to the origin of air. Here, interhemispheric differences as well as differences between continents and oceans will be considered. In particular, we discuss how the common AoA calculated relative to the whole PBL can be decomposed into its regional components. Second, we show that by using both AOFs and RMAs, an arbitrary tracer with specified linearly growing sources in every region can be analytically reconstructed at every space–time point in the atmosphere.

Although such a reconstruction strictly applies only for linear sources (see next section), we use this method to determine the global CO2 distribution with specified realistic spatial distributions and time evolution of the sources in the PBL as derived from the CarbonTracker dataset (Peters et al. 2007). We show that such a simplified forward model reproduces fairly well the CO2 distribution derived from a full chemistry transport model (CTM), especially if only the total column of CO2 is considered.

In the next section, we derive all necessary equations. Sections 3 and 4 discuss the regionally resolved seasonality of transport from the PBL to the TTL by extending the results presented in Orbe et al. (2015). In section 5, the simplified forward model of CO2 transport is presented. Finally, we discuss our results in section 6.

2. Airmass origin fractions and regionally resolved mean ages

The formal solution of the general transport equation for the mixing ratio of a conserved and passive tracer $\mu$ that is prescribed at the boundary $\Omega$ (e.g., Earth’s surface) can be written in terms of an age spectrum $G$, also called transit-time distribution (Hall and Plumb 1994; Waugh and Hall 2002):

$$\mu(\mathbf{r}, t) = \int_0^\infty \mu(\Omega, t - \tau) G(\mathbf{r}, \Omega, t - \tau) d\tau,$$  \hspace{1cm} (1)

where $\mu(\Omega, t - \tau)$ is the tracer mixing ratio at the boundary surface $\Omega$ time $\tau$ ago.

Now, we decompose the boundary $\Omega$ into a set of subregions $\Omega_i$ with $\sum \Omega_i = \Omega$, $i = 1, \ldots, n$, and with specified time series $\mu_i(t)$ in each region $\Omega_i$ and 0 elsewhere (see Fig. 1) such that

$$\mu(\Omega, t) = \sum_{i=1}^n \mu_i(t).$$  \hspace{1cm} (2)

In addition, defining $G_i$ inside $\Omega_i$ and 0 elsewhere allows us to write (Haine and Hall 2002)

$$G(\mathbf{r}, \Omega, t, t') = \sum_{i=1}^n G_i(\mathbf{r}, \Omega_i, t, t'),$$  \hspace{1cm} (3)

and, consequently, we can rewrite relation (1) as

$$\mu(\mathbf{r}, t) = \sum_{i=1}^n \int_0^\infty \mu_i(t - \tau) G_i(\mathbf{r}, t - \tau) d\tau,$$

where, from now on, we do not write the $\Omega$ dependence explicitly.

The term $G(r, t, t')$ can also be understood as a probability distribution function as it is the mass fraction of an air parcel that has left the boundary surface $\Omega$ time $\tau$ ago, hence a transit-time PDF.

![Fig. 1. The decomposition of the boundary $\Omega$ (such as that of Earth’s surface) into the $n$ subregions (such as continents and oceans), in which the passive tracer is specified in the form of time series $\mu_i(t)$.](image)
This means that $G$ is normalized to 1; that is,

$$\int_0^\infty G(\mathbf{r}, t, t - \tau) \, d\tau = 1. \quad (4)$$

With the special choice $\mu_i(t) = H(t - t_0)$ (with $H$ being the Heaviside step function) within each region $\Omega_i$, the AOFs $f_i$, $i = 1, \ldots, n$ can be defined as (Orbe et al. 2013)

$$f_i(\mathbf{r}, t) = \lim_{t_0 \to -\infty} \int_0^\infty H(t - t_0 - \tau) G_i(\mathbf{r}, t, t - \tau) \, d\tau = \int_0^\infty G_i(\mathbf{r}, t, t - \tau) \, d\tau. \quad (5)$$

Because of the normalization condition (4), the sum of the fractions equals 1 at every space–time point; that is,

$$\sum_{i=1}^n f_i(\mathbf{r}, t) = 1. \quad (6)$$

Note that such idealized origin tracers can be simply implemented into a CTM by setting $f_i$ to 1 inside $\Omega_i$ and 0 elsewhere in $\Omega$.

Furthermore, properly normalized transit-time PDFs for the individual source regions $\Omega_i$ can be defined as $G_i/f_i$. Their first moment over transit time $\tau$

$$\Gamma_i(\mathbf{r}, t) = \frac{1}{f_i} \int_0^\infty \tau G_i(\mathbf{r}, t, t - \tau) \, d\tau \quad (7)$$

defines the mean age of air with respect to the source region $\Omega_i$ or simply RMAs.

In particular, for a linear source function $\mu_i$, with

$$\mu_i(t) = a + bt, \quad a, b = \text{const}, \quad (8)$$

the relation

$$\mu_i(\mathbf{r}, t) = f_i(\mathbf{r}, t) \mu_i[t - \Gamma_i(\mathbf{r}, t)] \quad (9)$$

holds (for the derivation see below); that is, the time delay between the concentration $\mu_i$ at the space–time point $(\mathbf{r}, t)$ and the linearly increasing concentration at the source $\mu_i$ is equal to the mean age $\Gamma_i$.

The linearity of $\mu_i$ and the normalization condition of $G_i$ render the derivation of (9) very simple. Using the same arguments as in Hall and Plumb (1994), we obtain for the space–time distribution of the tracer $\mu_i$:

$$\mu_i(\mathbf{r}, t) = \int_0^\infty \mu_i(t - \tau) G_i(\mathbf{r}, t, t - \tau) \, d\tau = \int_0^\infty [a + b(t - \tau)] G_i(\mathbf{r}, t, t - \tau) \, d\tau = f_i(\mathbf{r}, t)[a + bt - b\Gamma_i(\mathbf{r}, t)] = f_i(\mathbf{r}, t)\mu_i[t - \Gamma_i(\mathbf{r}, t)].$$

It is also relatively easy to derive the spectrum of $\Gamma_i$ from a CTM. For this purpose, a linearly increasing tracer, as described above, has to be defined in each $\Omega_i$ region and set to zero elsewhere in the boundary layer. Thus, for the sum of the linear source functions $\mu_i$ [see Eq. (8)], we can write

$$\mu(\mathbf{r}, t) = \sum_{i=1}^n \mu_i(\mathbf{r}, t) = \sum_{i=1}^n f_i(\mathbf{r}, t)\mu_i[t - \Gamma_i(\mathbf{r}, t)], \quad (10)$$

where relation (9) was used. Because of

$$\mu(\mathbf{r}, t) = a + b[t - \Gamma(\mathbf{r}, t)]$$

$$= \sum_{i=1}^n f_i(\mathbf{r}, t)[a + b[t - \Gamma_i(\mathbf{r}, t)]] \quad (11)$$

the following relation connects $\Gamma$ with the $\Gamma_i$:

$$\Gamma = \sum_{i=1}^n f_i\Gamma_i. \quad (12)$$

Finally, after initializing a CTM covering the troposphere and stratosphere, a spinup period of around $m = 10, \ldots, 20$ years is expected until equilibrium with the boundary conditions has been reached (Orbe et al. 2013, 2015), such that all the $f_i$ and $\Gamma_i$ do not depend on the initialization time $t_0$:

$$f_i(\mathbf{r}, t, t_0), \Gamma_i(\mathbf{r}, t, t_0) \xrightarrow{>15\text{yr}} f_i(\mathbf{r}, t), \Gamma_i(\mathbf{r}, t). \quad (13)$$

A convenient way to achieve such a quasi-stationary state is to repeat the first year of the simulation $m$ times. Within such a perpetuum run, all species at the end of the year are interpolated on the first day of the same year. Although there is a discontinuous jump in the flow field due to such interpolation, this approach can significantly reduce numerical costs if Lagrangian CTMs are used [like Chemical Lagrangian Model of the Stratosphere (CLaMS) in this study; see next section]. In such a case, the same trajectories as calculated for the first year of the perpetuum run can also be used in the following $m$ years, reducing the total numerical costs by more than 80%.

In particular, the linearly increasing tracers $\mu_i$ have to be redefined at the end of each perpetuum period using the $f_i$ [see relation (5)]. Because of
\[
\mu(r, t - \Delta t) = \mu(r, t) - b \Delta t = \sum_{i=1}^{n} [\mu_i(r, t) - f_i(r, t) b \Delta t]
\]
with \(\Delta t\) denoting the perpetuum time period (here: 1 yr), we obtain the relation
\[
\mu_i(r, t - \Delta t) = \mu_i(r, t) - f_i(r, t) b \Delta t.
\]

3. Diagnostic of transport into the TTL: An example

As a CTM we use the 2005 perpetuum run of CLaMS (McKenna et al. 2002; Konopka et al. 2004; Pommrich et al. 2014) driven by the horizontal winds and diabatic heating rates (vertical velocities) derived from ERA-Interim (Dee et al. 2011). To resolve transport processes in the troposphere influenced by the orography and transport processes in the stratosphere where adiabatic horizontal transport dominates, the hybrid \(\sigma-\theta\) coordinate \(\zeta\) is used (where \(\sigma\) is a terrain-following coordinate and \(\theta\) is potential temperature) (Mahowald et al. 2002; Konopka et al. 2007). More details can be found in Pommrich et al. (2014).

All idealized tracers [i.e., those from which the \(f_i\) (AOFs) and \(\Gamma_i\) (RMAs) can be calculated] are set in the orography-following lower boundary of CLaMS defined by the condition \(0 \leq \zeta \leq 100\) K (i.e., within a layer covering roughly the first 1.5 km of the atmosphere above the ground). In the following, we consider this layer of the CLaMS air parcels as the simplest approximation of the PBL. At the upper boundary, all the air parcels in the layer between \(\zeta = 2200\) and 2500 K (around 0.1 hPa) are replaced by their initial configuration (same area of each air parcel depending on the resolution used) and all tracers are interpolated from their horizontal next neighbors in this layer (open boundary condition).

The 34 yr of CLaMS simulation of CO\(_2\) (from 1979 to 2012) extend between Earth’s surface and the mesosphere. Until the year 2000, a zonally symmetric lower boundary condition is used, which is derived from the NOAA/Climate Monitoring and Diagnostics Laboratory (CMDL) ground-based measurement network (Masarie and Tans 1995; Novelli et al. 2003) as described in Pommrich et al. (2014). For the 2000–12 period, the zonally resolved lower boundary was derived from the CarbonTracker dataset (Peters et al. 2007). Here the first five lowest levels of the CarbonTracker dataset (run CT2013B, available every 3 h; see https://www.esrl.noaa.gov/gmd/ccgg/carbontracker/), which roughly cover the PBL resolved by CLaMS, were vertically averaged and included in the CLaMS simulation as a 2D (longitude–latitude) lower boundary condition. In the following, the CO\(_2\) time–space evolution derived from such a CLaMS simulation is used as a reference—that is, as a proxy of a “true” CO\(_2\) distribution in the atmosphere.

To diagnose transport, in particular to determine the \(f_i\) and \(\Gamma_i\), CLaMS perpetuum runs for 2005 are carried out with a horizontal model resolution of 100 km (mean horizontal distance between air parcels) and vertical resolution of ~400 m around the tropopause. For sensitivity studies, results with reduced horizontal and vertical resolutions of 200 km and 800 m are shown. After each year of the 40-yr perpetuum run, the AOFs and RMAs are interpolated from the last day (31 December) to the first day (1 January) of the considered year whereas relation (15) is used for the linearly increasing tracers.

As shown later, we ensure in this way that the equilibrated state was reached; that is, all \(f_i\) and \(\Gamma_i\) do not depend on the initialization time \(t_0\). Note that our way of calculating AOFs and RMAs from a perpetuum run (instead of from a sufficiently long transient run) neglects some interannual variability of transport such as that due to the El Niño–Southern Oscillation (ENSO) or due to the quasi-biennial oscillation (QBO). Especially air masses older than 1 yr (perpetuum cycle) are affected by our approximation, although they are of minor importance for our analysis (shown later).

An example of AOFs and RMAs, calculated for 15 December 2005, can be seen in Fig. 2. Here, 36 almost-equal source regions are defined as a regular grid covering Earth’s surface (black grid; note that boxes covering the polar caps are slightly larger than all other boxes in the tropics and extratropics). The TTL is considered as a destination region over which all \(f_i\) and \(\Gamma_i\) are averaged (thick black box). For better comparison with Orbe et al. (2015), the TTL is defined as a domain between 20°S and 20°N and between 100–70 hPa.

As expected, the largest fraction of air in the TTL originates from the tropical belt between 20°S and 20°N (in total more than 60%) with the highest contribution from the Maritime Continent, tropical Pacific, and Indian Ocean. On the other hand, the youngest air (i.e., the fastest mean transport) occurs over the tropical/subtropical Pacific, whereas the oldest air originates from the southern polar region. Note that although the highest values of AOFs are located around the equator there is a stronger hemispheric asymmetry in the distribution of RMAs with
much older air from the southern than from the northern high latitudes.

It is important to note that in order to obtain results that are independent of the initialization time of the artificial tracers, a quasi-stationary state has to be reached. As an example, Fig. 3 shows how the values of \( f_{10} \) and \( \Gamma_{10} \) (tenth region within \( 0^\circ-20^\circ S, 0^\circ-60^\circ E \); red dashed box in Fig. 2) converge to such independent values after 40 yr of the perpetuum simulation (note that \( f_{10} \) and \( \Gamma_{10} \) converge to their final values after \( \sim 8 \) and \( \sim 15 \) perpetuum years, respectively). Then, initial conditions can be ruled out and \( f_i \) and \( \Gamma_i \) can be understood as diagnostics of pure transport.

4. Seasonality of regionally resolved mean ages in the TTL

First, we compare our results for AOFs with similar results published by Orbe et al. (2015) (although a different CTM and different winds were used) and define the source and destination regions as shown in Fig. 4. Following Orbe et al. (2015), three source regions in the PBL (0–1.5 km) are considered: Southern Hemisphere (SH; \( 90^\circ-10^\circ S \); green), tropics (\( 10^\circ S-10^\circ N \); red), and the Northern Hemisphere (NH; \( 10^\circ-90^\circ N \); cyan). Beyond the TTL as a destination region, we also consider two additional regions in the extratropical troposphere (TR): TR–SH (800–700 hPa, \( 90^\circ-50^\circ S \)) and TR–NH (800–700 hPa, \( 50^\circ-90^\circ N \)).

The seasonality of the respective \( f_i \) and \( \Gamma_i \) for all three destination regions (TTL, TR–SH, and TR–NH) is shown in Fig. 5. The top panel of Fig. 5a shows the seasonalities of the mass fractions \( f_i \), which are roughly the same as those discussed in Orbe et al. (2015) (see their Fig. 2a); that is, the composition of the TTL is dominated (by more than \( \sim 60\% \)) by the air from the tropical belt between \( 10^\circ S \) and \( 10^\circ N \) and with a maximum (minimum) around June or July (November).

The tropical belt also determines the mean age in the TTL as can be inferred from the bottom panel of Fig. 5a: according to Eq. (12), the mean age of the total Earth’s surface (black) can be decomposed into the tropical contribution (red) as well as the extratropical contributions of the Southern (green) and Northern (blue) Hemispheres. Note that the black lines and the red lines are very similar, indicating that the mean age relative to the total Earth’s surface is almost the same as the mean age relative to the tropical belt. It should be mentioned that the youngest air from the extratropical Southern (Northern) Hemisphere is expected around April (December) with a respective mass fraction of \( \sim 20\% \) (\( \sim 40\% \)). The higher contribution of the extratropical air from the NH during December than from the SH during April is a result of the delayed influence of the Hadley cell with the equatorward branch being stronger during the summer in the NH than during the winter in the SH.

Now, we perform the same type of analysis for the polar tropospheric air between 700 and 800 hPa (see TR–SH and TR–NH regions in Fig. 4). The respective seasonalities of \( f_i \) and \( \Gamma_i \) (Figs. 5b and 5c) quantify fairly well the asymmetries in hemispheric and the inter-hemispheric transport. First, tropical air (red) reaches the TR–NH region more effectively than the TR–SH region with the fastest transport in the winter hemisphere because of more effective quasi-isentropic stirring by tropospheric eddies during the winter than during the summer and in the NH than in the SH. Furthermore, the mass fraction of the NH PBL in the SH polar troposphere amounts to \( \sim 6\% \) [blue curve in Fig. 5b (top)]. The reverse contribution (i.e., that of the SH PBL in the NH polar troposphere) is roughly 3 times smaller [green curve in Fig. 5c (top)]. The comparison of the regional mean ages reveals that, on average,
The fastest transport from the NH PBL to the SH polar troposphere can be diagnosed around October and vice versa around May.

The values of the mean age for the transport from the extratropical NH to the polar SH troposphere can also be compared with the mean age derived from the SF$_6$ observations (Waugh et al. 2013). As SF$_6$ is emitted predominantly in NH midlatitudes and its growth rate is nearly linear, the time lag between the SF$_6$ mixing ratio at a given location and that at the NH midlatitude...
surface provides an estimate of the mean age from the NH surface. Waugh et al. (2013) report values of around 16–18 months for the AoA of SF₆ at 60°S (see their Fig. 3), which roughly correspond to our estimate of around 15 months (see blue line in Fig. 5b) (bottom). However, the seasonality of AoA in TR–SH is very similar to that derived from SF₆ observations at Cape Grim (Tasmania, 40.7°S) and at the South Pole (Antarctica, 90°S) as described in Waugh et al. (2013).

Note that the analysis of AOFs and RMAs does not allow any conclusions to be drawn about the possible pathways of transport. Orbe et al. (2016) have recently shown that the transit-time distribution (TTD) (i.e., the full age spectrum) provides much more detailed information on transport from the NH midlatitude surface. In particular, huge differences in the seasonality of the pathways were diagnosed although the respective differences in the mean ages were much smaller. It should be also emphasized that all the diagnostic results discussed here and in other studies strongly depend on the quality of the wind fields used to run the CTM and how unresolved processes such as convection, gravity waves, or mixing are parameterized in the model.

Finally, the same type of analysis, but for the source regions defined by all continents and all oceans on Earth, is shown in Fig. 6. In the top panel, only the mass fraction of the continents \( f \) (red) is shown because the contribution of the oceans \((1 - f)\) follows from the normalization condition. The dashed line denotes the geometric percentage of continents of 29.7%. Thus, only during SON is the contribution of the continents slightly higher (2%–3%) than a simple geometric estimate. The analysis of respective
mean ages shows that the mean age of the continental/oceanic air only differs slightly from the mean age calculated relative to the whole Earth’s surface. Furthermore, the strongest contribution of the continents during the SON season is accompanied by the fastest mean transport if compared with the oceans, although the differences are less than 1 month. All these seasonalities depend only weakly on the chosen year (here 2005) or on the method how the equilibrated state was reached (perpetuum versus transient run), as confirmed for the CLaMS low-resolution case.

5. A simplified forward model

Now we apply relation (10) to reconstruct the temporal evolution of the CO2 distribution in the whole atmosphere. The use of relation (10) can also be understood as a (simplified) forward model propagating CO2 from the PBL into the whole atmosphere. Because we can derive the true CO2 distribution from a CTM (here CLaMS) and compare this distribution with that derived from Eq. (10), the quality of this approximation can be verified in this way.

The regions are defined either by a regular longitude–latitude (Xn/Ym) grid with roughly the same area of every (n, m)th grid cell or by defining different areas for continents and oceans (Cn/Om, where n and m are the numbers of continental and oceanic regions, respectively), known as nested grids (see Fig. 7). Thus, the following grids will be used: X6/Y6, X12/Y12, C1/O1, C17/O18, and C78/O18 with 36, 124, 2, 35, and 96 regions, respectively.

Thus, using relation (10), \( \mu(r, t) \) denotes a CO2 mixing ratio that is reconstructed from the mixing ratios \( m_i \) in the PBL, which are specified over the elapsed time and averaged over each region \( i \). Furthermore, the \( f_i \) and \( G_i \) contain information about the amount and time scale of tracers transported from the region \( i \) to the considered space–time \( (r, t) \) and are derived from the 2005 perpetuum run with CLaMS.

An example of such a reconstruction (calculated for 15 December 2006 by using the C78/O18 grid) is shown in the right-hand column of Fig. 8. The left-hand column shows the true CO2 distribution as derived from the full CLaMS simulation without dividing the PBL into regions.

In particular, in the top two panels, the CO2 mixing ratio in the PBL (i.e., in the lowest layer of CLaMS) can be seen with values derived from the CarbonTracker dataset (left) and after averaging this field over the regions according to the relation (10). Note that \( \mu_i [t - G_i (r, t)] \) in Eq. (10) denotes CO2 mixing ratios at the surface shifted to the past by the mean age \( \Gamma_i \) at the considered space–time point \( (r, t) \) and averaged over the region \( i \). Because we cannot show all the PBL values in the past, here only the values for 1200 UTC 15 December 2006 are plotted.
Fig. 8. (left) Full transport of CO₂ with CLaMS vs (right) simplified transport following relation (10). (top) Specified CO₂ distribution in the PBL (left) as derived from the CarbonTracker dataset and (right) as averaged over the grid boxes in order to obtain input for the simplified transport according to Eq. (10). (top middle),(bottom middle) Transported CO₂ as derived (left) directly from CLaMS and (right) by the use of the forward model (10). The parameters \( f_i \) and \( G_i \) are calculated from a 15-yr perpetuum run with CLaMS. (bottom) The column-averaged CO₂ (XCO₂) is a proxy for the data that can be expected from a satellite. All panels are examples for 1200 UTC 15 Dec 2006.
The second and third rows in Fig. 8 depict the respective snapshots (i.e., for the same date) in two different pressure layers (600–700 and 120–150 hPa). Once again, whereas in the left-hand column, the CO2 mixing ratios in CLaMS air parcels are calculated from the full Lagrangian transport (advection + mixing), the right-hand column uses Eq. (10) with precalculated AOFs $f_i$ and RMAs $\Gamma_i$. In the bottom row, the column-averaged $XCO_2$ is shown first by interpolating the irregular grid of Lagrangian air parcels on a regular pressure grid and then using the relation

$$XCO_2 = \frac{\int_{0}^{z} N_{CO_2}(z) \, dz}{\int_{0}^{z} N_{air}(z) \, dz}$$

with $N_{CO_2}(z)$ and $N_{air}(z)$ denoting the number density of CO2 and of air, respectively ($z$ is log-pressure altitude).

Note that although differences in the CO2 distribution in the PBL used in both procedures are significant (cf. top panels of Fig. 8), the differences in the respective XCO2 are much smaller. Figure 9 depicts such relative differences in XCO2 derived from CLaMS simulations with the highest nested resolution of the regions (C78/O18). We conclude that by using Eq. (10) the differences in XCO2 relative to a resolved full transport are smaller than 1% (i.e., they are on the order of the accuracy of current and future satellite instruments measuring XCO2). It is also worth noting that a sharp edge around 20°N in the relative differences shown in Fig. 9 is a result of the definition of the regions (see top-right panel in Fig. 8), which has still some potential for improvement.

Finally, we discuss how the performance of our approach depends on the grid resolution and on the choice of the mean ages $\Gamma_i$. In the left panel of Fig. 10, the vertically resolved differences (root-mean-square deviations in every CLaMS layer) between the results of the full and simplified transport calculations are shown. In the left panel, only one mean age $\Gamma$ calculated for the...
whole surface of Earth is used in Eq. (10) (i.e., \(\Gamma_i = \Gamma\)), whereas in the right panel, all the regional \(\Gamma_i\) are taken into account.

It can be seen that below 500 hPa the C78/O18 model configuration (105 regions) performs the best with mean differences smaller than 1.5 ppmv. The use of regionally resolved \(\Gamma_i\) improves the \(\text{CO}_2\) reconstruction by more than 50%. Note that taking into account more continental regions than oceanic regions helps to keep numerical efforts low (105 regions of the C78/O18 configuration versus 124 regions of the X12/Y12 regular grid) and also reduces the errors below 500 hPa by more than 50%. By using a transient instead of a perpetuum run (case C17/O18), the results shown in Fig. 10 are exactly the same below 200 hPa with no significant improvement above this level, consistent with transit times usually smaller than 1 yr below this level (not shown).

6. Conclusions

Starting from the airmass origin fractions (AOFs) defining the contribution of different regions on Earth to the composition of air at a given space–time point, we extended this analysis by considering the regionally resolved mean ages (RMAs) characterizing the mean transport from the regions to the space–time point considered. We showed how this additional diagnostic allows a more detailed characterization of transport.

In particular, the mean age of air (AoA), calculated relative to the PBL of the whole Earth, can be decomposed into its regionally resolved components (12). For example, the seasonality of the AoA in the TTL is the same as for the air originating in the tropical belt between 10°S and 10°N (oldest air around August or September, \(~60\%\) contribution) whereas the seasonalities of the air originating south of 10°S (north of 10°N) peak 1–2 months earlier (later), both with a contribution of \(~20\%\). In addition, the asymmetry of interhemispheric exchange could be quantified showing a faster mean transport from the SH and tropics into the lower NH polar troposphere than vice versa. Furthermore, the seasonality of mean ages from the continents and oceans is very similar with the youngest air from December to May and the oldest air from June to September.

We have also shown how knowledge of the time evolution of the AOFs and RMAs at every grid point of the model allows us to reconstruct a passive tracer with known linear sources everywhere in the atmosphere. The AOFs and RMAs can be easily calculated from the pure transport part of a CTM (i.e., the chemistry modules can be switched off). Typically CTMs are driven by reanalysis winds (here ERA-Interim), which extend over a few decades and make the perpetuum runs (as used in this paper) only necessary for the first year of the simulation. Furthermore, the CTM has to be run only once to determine the transport properties (i.e., the AOFs and RMAs) and then the simplified forward model can be applied to any tracer given its concentration at the surface.

Such a simplified model was applied and validated by studying \(\text{CO}_2\) propagation from Earth’s surface into the atmosphere extending up to the stratopause. Currently, using satellite observations such as those of the European Scanning Imaging Absorption Spectrometer for Atmospheric Chartography (SCIAMACHY), Japan’s \(\text{Greenhouse Gases Observing Satellite}\) (GOSAT), or the recently launched U.S. \(\text{Orbiting Carbon Observatory}\) (OCO), only the column of \(\text{CO}_2\) or XCO2 (i.e., the mean mixing ratio of \(\text{CO}_2\) averaged over the column) can be derived. The differences between the full and simplified transport, especially in terms of column-averaged XCO2, are smaller than 1% (i.e., on the order of the accuracy of the satelliteborne measurements).

Thus, the forward model presented offers a simple framework for the inverse modeling of \(\text{CO}_2\) also known as the top-down approach (Nisbet and Weiss 2010). In particular, using this approach, the sensitivity of XCO2 with respect to the distribution of \(\text{CO}_2\) sources, such as their spatial inhomogeneities or their diurnal and seasonal cycles, can be analyzed in order to find out which properties of XCO2 variability reflect anthropogenic footprints. A conceptually similar type of analysis was discussed in Stohl (2006) where the sensitivity of Arctic pollution to different midlatitude source regions was quantified in terms of the Arctic age (i.e., the time air resides continuously north of 70°N).

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