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Key Points:
- Data assimilation improves the TIL in modern systems
- Direct analysis of 4D-Var increments
- ERA-Interim and ECMWF operational forecast system compared to GPS-RO

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Tropopause sharpening by data assimilation

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Abstract Data assimilation was recently suggested to smooth out the sharp gradients that characterize the tropopause inversion layer (TIL) in systems that did not assimilate TIL-resolving observations. We investigate whether this effect is present in the ERA-Interim reanalysis and the European Centre for Medium-Range Weather Forecasts (ECMWF) operational forecast system (which assimilate high-resolution observations) by analyzing the 4D-Var increments and how the TIL is represented in their data assimilation systems. For comparison, we also diagnose the TIL from high-resolution GPS radio occultation temperature profiles from the COSMIC satellite mission, degraded to the same vertical resolution as ERA-Interim and ECMWF operational analyses. Our results show that more recent reanalysis and forecast systems improve the representation of the TIL, updating the earlier hypothesis. However, the TIL in ERA-Interim and ECMWF operational analyses is still weaker and farther away from the tropopause than GPS radio occultation observations of the same vertical resolution.

1. Introduction

The tropopause inversion layer (TIL) consists of a sharp temperature inversion and a corresponding maximum in static stability right above the thermal tropopause [*Birner et al.*, 2002] that is present globally [*Birner*, 2006; *Grise et al.*, 2010]. The high static stability values within the TIL can affect the dispersion relations of atmospheric Rossby or inertia-gravity waves [*Birner*, 2006; *Grise et al.*, 2010] and inhibit the cross-tropopause exchange of chemical compounds by preventing vertical motion, since stability correlates with trace-gas gradients [*Hegglin et al.*, 2009; *Kunz et al.*, 2009; *Schmidt et al.*, 2010].

The TIL is a fine-scale feature whose properties can only be captured by data of high vertical resolution (~100 m), i.e., GPS radio occultation (GPS-RO) by satellites and high-resolution radiosonde measurements. Atmospheric models are very limited in this sense, generally having a vertical resolution near the tropopause of around 1 km. *Hegglin et al.* [2010] and *Gettelman et al.* [2010] compared the TIL in various models within the Chemistry Climate Model Validation project 2 (CCMVal2). They degraded the vertical resolution of GPS-RO observations to the models' standard pressure levels and found that even after accounting for vertical resolution differences, the modeled TILs were always farther away from the tropopause and generally weaker than the TIL retrieved from degraded observations.

Birner et al. [2006] investigated the TIL in two data assimilation systems, the National Centers for Environmental Prediction/National Center for Atmospheric Research (NCEP/NCAR) reanalysis [*Kalnay et al.*, 1996] and the Canadian Middle Atmosphere Model assimilating observations (CMAM+DA) [*Polavarapu et al.*, 2005]. The atmospheric models in both systems have a vertical resolution of roughly 1 km near the tropopause, and both systems use three-dimensional variational (3D-Var) data assimilation. *Birner et al.* [2006] found that the TIL from the free-running CMAM was stronger than the TIL from CMAM with data assimilation and the NCAR reanalysis and showed how data assimilation weakened the TIL in CMAM immediately after being switched on. Therefore, *Birner et al.* [2006] suggested that data assimilation smooths out the sharp gradients that lead to the formation of the TIL. It has to be pointed out that neither of those systems assimilated GPS-RO data.

Recently, modern reanalyses have been used to study the TIL, as is the case in *Gettelman and Wang* [2015] who produced a set of TIL diagnostics from ERA-Interim [*Dee et al.*, 2011] and *Wargan and Coy* [2016] who showed TIL enhancement during a sudden stratospheric warming in Modern-Era Retrospective Analysis for Research and Applications version 2 (MERRA-2) [*Molod et al.*, 2015]. The reanalyses used in these studies include innumerable improvements from those analyzed by *Birner et al.* [2006]: model resolution has increased, bias correction has become more sophisticated, as well as the parameterizations (clouds, convection, gravity waves, etc.), the data assimilation procedures have evolved (e.g., four-dimensional variational data assimilation, 4D-Var [*Rabier et al.*, 2000], has been implemented in ERA-Interim), and large amounts of high-resolution GPS-RO profiles (especially from the COSMIC satellite mission [*Anthes et al.*, 2008]) are assimilated, among many other improvements that result in a better representation of the atmosphere.

Our goal is to test whether the hypothesis of *Birner et al.* [2006], that data assimilation smoothes out the TIL, is still valid in newer systems. To achieve this, we will study the TIL and how it is affected by data assimilation in ERA-Interim and a more recent version of the European Centre for Medium-Range Weather Forecasts (ECMWF) operational forecast model. The latter has greater horizontal and vertical resolutions and is used to test whether the effect of data assimilation is still the same despite the different versions of the assimilating model. Our results show TIL improvement by data assimilation with very similar structures in both systems. As discussed in the previous paragraph, there are innumerable differences between the assimilation systems in *Birner et al.* [2006] and modern ones, thus specifying which factors in particular are responsible for the better representation of the TIL is beyond the scope of our study and requires further research and experiments.

As a first step, we will show the TIL in the ERA-Interim reanalysis and the ECMWF operational analyses, comparing both to the TIL from GPS-RO observations degraded to the corresponding model levels. Secondly, we investigate the effect of data assimilation by analyzing the 4D-Var analysis increments, i.e. the difference in the model states before and after data assimilation, in terms of static stability. This two-step approach is necessary to discern how data assimilation affects the TIL, since the 4D-Var increments have to be subtracted from the analysis states (obtained at the first step) to enable the calculation of the static stability structures in both systems before data assimilation was done (see section 2 for methodology details).

The time period for our analysis is January 2010. In this month, our results show a TIL representative of a Northern Hemisphere's winter climatology in both the ERA-Interim reanalysis and ECMWF operational (see section 3) and systematic structures in the mean increments of static stability across all latitudes in both data assimilation systems (see section 4), indicating that these results are robust.

We describe the data used in this study, the procedure to degrade high-resolution GPS-RO profiles to the models' pressure levels, and how the increments in static stability are calculated, in section 2. We show how the TIL is represented in the ERA-Interim reanalysis and the ECMWF forecast model compared to degraded observations in section 3. The effect of data assimilation on the TIL strength is discussed in section 4, and we summarize the main conclusions in section 5.

2. Data and Methods

2.1. GPS-RO Observations, the ERA-Interim Reanalysis, and the ECMWF Operational Forecast Model

We use temperature profiles from GPS radio occultation (GPS-RO) measurements made by the COSMIC satellite mission [*Anthes et al.*, 2008]. The profiles have a vertical resolution of 100 m and extend from the surface up to 40 km altitude; which is similar to high-resolution radiosonde measurements but with the advantage of weather independence, a much higher measurement density (around 2000 profiles per day), and global coverage. The assimilation of GPS-RO observations has had a major impact in both reanalysis and numerical weather prediction systems, having improved the representation of upper tropospheric and stratospheric temperatures: although GPS-RO data are not the largest observation source (satellite radiances), they do have the highest assimilation rate among data sets in the ERA-Interim reanalysis [*Poli et al.*, 2010] (60–65% of the observations are assimilated, compared to a 50% rate of assimilation for radiosondes), and GPS-RO data are among the top influencers on analyses and forecasts in the ECMWF numerical weather prediction system, especially between 10 and 20 km altitude [*Cardinali and Healy*, 2014].

The ERA-Interim reanalysis [*Dee et al.*, 2011] uses the ECMWF operational forecast model from early 2007 (IFS Cycle 31r2), which has 60 vertical model levels with the top at 0.1 hPa (~65 km) altitude, a vertical resolution of 700–800 m near the extratropical tropopause, and a T255 (~80 km) horizontal grid.

We also analyze data from a newer version of the ECMWF operational weather forecast system valid in January 2010 (IFS Cycle 35r3), which has 91 vertical model levels with the top at 0.01 hPa (~80 km) altitude, a 400–500 m vertical resolution near the tropopause, and a T1279 (~16 km) horizontal grid. This allows us to compare the results from ERA-Interim reanalysis to a newer version of the same atmospheric model. Since the operational analysis has better vertical resolution, it should capture the gradients that lead to the TIL better than ERA-Interim, though the main purpose of this comparison is to test whether the effect of data assimilation on the TIL is changed or not in the two versions of the same assimilating model. Both data assimilation systems use four-dimensional variational assimilation (4D-Var) [e.g., *Rabier et al.*, 2000] to fit their atmospheric models to the observations (see *European Centre for Medium-Range Weather Forecasts* (ECMWF) [2007a] for an in-depth description).

We use the following 6-hourly output variables from the ECMWF reanalysis and operational systems: surface geopotential, surface pressure, the hybrid coordinates of the model levels (L60 in the reanalysis, L91 in the operational system), and the temperature and specific humidity at the model levels. Also, we use the 4D-Var increments (the difference in the model states before and after data assimilation) of surface pressure, temperature, and specific humidity.

From the surface pressure and the hybrid levels, the model levels' pressure can be calculated, and combining the information of surface geopotential and the model levels' pressure, temperature, and specific humidity, the geopotential height of each level can be obtained. For a detailed description of the equations used for this in the ECMWF reanalysis and operational atmospheric models, see the vertical discretization chapter in the IFS documentation of *ECMWF* [2007b] (developed after *Simmons and Burridge* [1981]). All data sets are analyzed for January 2010. As discussed in the introduction, we suggest that 1 month of data is enough given the systematic and similar structures found in both data assimilation systems, regarding 4D-Var increments and differences between the models and degraded GPS-RO observations (see sections 3 and 4).

2.2. Degradation of GPS-RO Profiles Onto Model Levels

For each GPS-RO profile, we take the grid point and time nearest to the observation and retrieve the pressure of each hybrid model level (L60 for the reanalysis, L91 for the operational system). Each GPS-RO temperature profile comes together with height and pressure information, and the degraded GPS-RO profile is simply a subsample with the information of the 60 (or 91) levels with pressure closest to the reanalysis (or operational) model levels' pressures. Our method is very similar to the one used by *Gettelman et al.* [2010] and *Hegglin et al.* [2010], but instead of standard pressure levels, we use the local pressure of the models' hybrid levels, allowing variability in space and time.

2.3. TIL Calculations

Using the temperature, height, and pressure profiles in ERA-Interim, the ECMWF operational analysis (calculated in section 2.1), and the GPS-RO observations degraded to the same vertical grid as the atmospheric models (see section 2.2), we calculate static stability vertical profiles as the Brunt-Väisälä frequency squared, i.e., $N^2(s^{-2}) = g/\Theta \cdot \partial\Theta/\partial z$, where g is the gravitational acceleration and Θ the potential temperature. Profiles where the tropopause cannot be found and those with temperature < -150°C or >150°C or $N^2 > 100 \times 10^{-4}\ s^{-2}$ (unrealistic values that we would like to avoid) are excluded, amounting to less than 1% of the profiles.

We define tropopause height (TP_z) as the height of the lapse-rate tropopause following the World Meteorological Organization criterion [*World Meteorological Organization*, 1957] and use it as the reference level for averaging, to obtain tropopause-based zonal-mean N^2 profiles, as in *Birner et al.* [2002]. We calculate the TIL strength as the maximum static stability value (N^2_{max}) in the first 3 km above the tropopause (although our algorithm finds it most often in the first kilometer). This TIL strength measure has the advantage of being independent of its distance from the tropopause and is commonly used [*Birner et al.*, 2006; *Wirth and Szabo*, 2007; *Erler and Wirth*, 2011; *Pilch Kedzierski et al.*, 2015].

2.4. Obtaining the Prior States With 4D-Var Increments

To obtain prior values for ERA-Interim and the ECMWF operational system, the 4D-Var increments of surface pressure, temperature, and specific humidity are subtracted (each iteration at a time, backward) from the analysis (or posterior) values. After each subtraction, the calculations from sections 2.1 and 2.3 are done again, obtaining the N^2 profiles and N^2_{max} values in the atmospheric models before each iteration of the data assimilation procedure. In ERA-Interim reanalysis two iterations are done during the 4D-Var procedure, whereas three iterations are used in the ECMWF operational system.

Note that while the analysis output variables are 6-hourly (00, 06, 12, and 18 UTC), the 4D-Var assimilation is done over 12 h windows, so the increments are also 12-hourly (09 and 21 UTC for the operational system; 03 and 15 UTC for ERA-Interim). The increments are subtracted from the immediately afterward 6-hourly analyses.

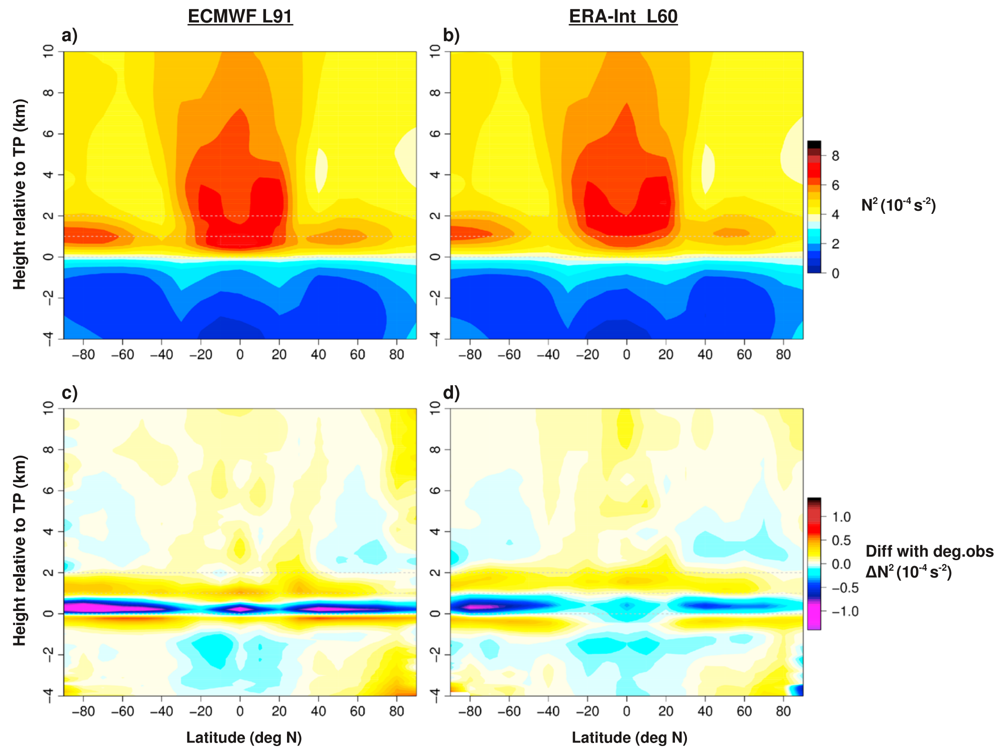

Figure 1. Latitude-height sections of tropopause-based zonal-mean N^2 in (a) the ECMWF L91 forecast model and (b) the ERA-Interim reanalysis. The bottom row differences from observations degraded to (c) the pressure of ECMWF's 91 model levels and (d) the pressure of ERA-Interim's 60 model levels. Averaged for January 2010. For orientation, grey dashed lines denote the tropopause and +1/+2 km.

This way, we have the same TIL diagnostics of the following data sets: the analysis output from ERA-Interim and the ECMWF forecast model, which are produced after the 4D-Var data assimilation (see sections 2.1 and 2.3), GPS-RO observations with their vertical resolution equaled to the atmospheric models' (sections 2.2 and 2.3), and the model states prior to data assimilation and in between each iteration.

3. The TIL in ECMWF Forecasts and Reanalysis

Before analyzing the effect of data assimilation on the TIL, this section shows how the TIL is represented in the ERA-Interim reanalysis [*Dee et al.*, 2011] and the newer, higher-resolution ECMWF operational analysis, comparing it to the TIL from degraded GPS-RO observations, which eliminates vertical resolution as a source of differences.

The Figures 1a and 1b show the zonal-mean, tropopause-based N^2 profiles at all latitudes for the ECMWF operational analysis and ERA-Interim, averaged over January 2010. Both panels show N^2 maximized near 1–1.5 km above the tropopause at all latitudes, meaning that the TIL is captured globally in both the operational system and the ERA-Interim reanalysis. The TIL from Figures 1a and 1b resembles the observed climatological winter structure of the TIL, with relative maxima in the winter (Northern Hemisphere) midlatitudes and the summer (Southern Hemisphere) pole [*Birner*, 2006; *Grise et al.*, 2010] and higher N^2 values near the equator, which are present all year round, [*Grise et al.*, 2010] due to the large negative lapse rate in the background temperature profile of the equatorial stratosphere.

Comparing the ECMWF operational system (L91, Figure 1a) to ERA-Interim (L60, Figure 1b), the first has a slightly stronger TIL, situated a few hundreds of meters closer to the tropopause. Given that the operational system in 2010 had a better vertical resolution than the model version used in ERA-Interim (see section 2.1), its ability to capture sharper gradients near the tropopause is straightforward. But when the operational system and ERA-Interim are compared to GPS-RO observations degraded to their respective vertical resolutions (Figures 1c and 1d), a very similar pattern appears globally: relative to the degraded observations, both ECMWF operational and ERA-Interim have lower N^2 values in the layer 0–1 km above the tropopause

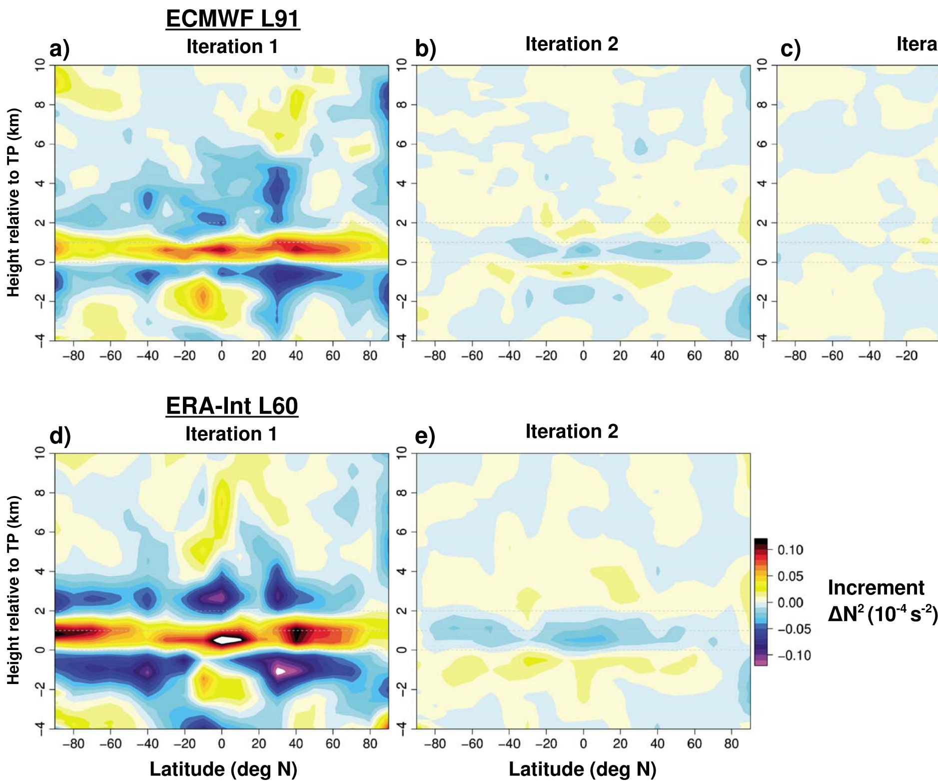

Figure 2. Zonal-mean, tropopause-based N^2 increments over successive iterations of the 4D-Var assimilation procedure for (a–c) the ECMWF L91 forecast model and (d, e) the ERA-Interim reanalysis. Averaged for January 2010. For orientation, grey dashed lines denote the tropopause and +1/+2 km.

(between -0.5 and -1×10^{-4} s^{-2}, blue-purple colors) and higher values in the layer 1–2 km above the tropopause (between 0.25 and 0.5×10^{-4} s^{-2}, yellow-orange colors). This pattern indicates that the TIL in both the 2010 ECMWF operational analysis and ERA-Interim is farther away from the tropopause than in the degraded GPS-RO observations. The negative differences in the layer 0–1 km above the tropopause (blue in Figures 1c and 1d) are about double that of the positive difference in the layer 1–2 km above the tropopause; this suggests that the TIL of the degraded observations is still slightly stronger in both cases (which is confirmed in section 4, Figure 3). We also find that the ECMWF operational analysis and ERA-Interim have higher N^2 in the uppermost troposphere, especially in the extratropics (Figures 1c and 1d), meaning that the transition from tropospheric values to the higher N^2 in the TIL is less sharp than in degraded observations.

To summarize this section, both ERA-Interim and the ECMWF operational system have a TIL slightly weaker and farther away from the tropopause than expected from GPS-RO observations with the same vertical resolution, a difference which persists across all latitudes and has a very similar structure in both systems (Figures 1c and 1d). *Gettelman et al.* [2010] and *Hegglin et al.* [2010] reported a similar tendency in free-running atmospheric models from CCMVal2 [see *Gettelman et al.*, 2010, Figure 12] with the TIL shifted away from the tropopause and generally weaker than degraded observations. Although to a much lower degree, we see here that this issue is also present in ERA-Interim and the ECMWF forecast system.

4. The Effect of Data Assimilation on the TIL Strength

Figure 2 shows the 4D-Var increments in terms of N^2, calculated as tropopause-based zonal means for January 2010. The largest increments occur in the first iteration of the 4D-Var data assimilation process for both the ECMWF operational system (Figure 2a) and ERA-Interim [*Dee et al.*, 2011] (Figure 2d). The first iteration (Figures 2a and 2d), on average, increases N^2 in the first 1.5 km above the tropopause at all latitudes and decreases N^2 above and below that layer. The second iteration (Figures 2b and 2e) has the opposite tendency but at only about one fourth of the magnitude, counteracting a small part of the positive increments of the first iteration. The operational system's third iteration (Figure 2c) has no coherent structures.

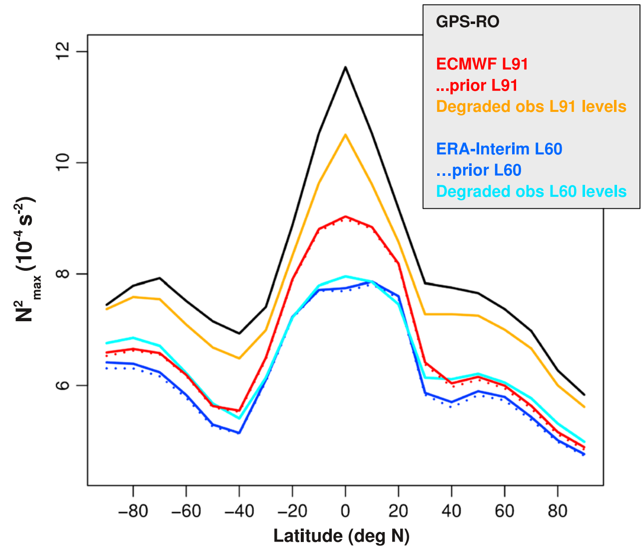

Figure 3. Zonal-mean TIL strength over all latitude bands measured as N^2_{max}. The color lines corresponding to the different data sets are shown in the top right corner. Averaged for January 2010.

Since the overall effect of the 4D-Var data assimilation process is the sum of all iterations, the net increment in N^2 in the first 1.5 km above the tropopause at all latitudes is an increase of $\sim 0.1 \times 10^{-4}$ s^{-2} for the operational system and $\sim 0.07 \times 10^{-4}$ s^{-2} for ERA-Interim. Although the magnitude is slightly different in the two versions of the assimilating model, the latitude-vertical structures are nearly the same. The N^2 increments have relative maxima where the TIL is stronger during NH winter: near the South Pole, the NH midlatitudes, and at the equator. Although the N^2 increments amount to only about 1.3 % of the actual TIL strength, the timescale of assimilation (12 h) is fast relative to the dynamics associated with the TIL, and an atmospheric model initiated with a TIL as in Figure 1 cannot drift and smooth out the TIL significantly in a 12 h period. Figure 2 demonstrates that without data assimilation, both versions of the ECMWF atmospheric model tend toward a weaker N^2 in the TIL region. The TIL being farther away from the tropopause in the data assimilation systems compared to degraded GPS-RO observations (Figure 1) cannot be explained by the 4D-Var increments in Figure 2, since they rather act to slightly compensate this bias.

We conclude from Figure 2 that the 4D-Var data assimilation systematically increases N^2 in the TIL region at all latitudes, with the TIL prior to the data assimilation steps being consistently slightly weaker in both systems. This is the main result of our study, and it contradicts the hypothesis of *Birner et al.* [2006] that the data assimilation process smoothes out the TIL. Our results show that when high-resolution data (GPS-RO) are assimilated into models with better vertical resolution (ECMWF operational and ERA-Interim) with the most advanced data assimilation techniques (4D-Var), the representation of the TIL is improved. However, we cannot discern which factor contributes the most, e.g., quantifying how much of the improvement in the TIL representation comes from assimilating GPS-RO in contrast with the update from 3D-Var to 4D-Var is impossible nowadays because there is no reanalysis using 3D-Var and GPS-RO data, neither one using 4D-Var without GPS-RO. Additional experiments with one model version (and varying observational input and assimilation techniques) could be carried out in order to point out the key factors.

Nevertheless, from Figures 1 and 2 we can see that varying horizontal and vertical resolutions do not affect the main results in two versions of the same assimilating model: vertical resolution is undoubtedly a limiting factor to resolve the TIL, but the differences between the analyses and degraded observations in ERA-Interim and ECMWF operational have very similar structures (Figure 1). In the case of the N^2 increments, their structures are also similar, and the TIL is enhanced in both systems (Figure 2).

Figure 3 summarizes the findings of our study, showing the TIL strength scores over all latitudes, calculated as N^2_{max} (a TIL strength measure independent of the distance from the tropopause; see section 2.3) for ERA-Interim and the operational system (blue and red lines, respectively), their states prior to data assimilation (dotted lines of the same colors), and the observations degraded to the same vertical resolution (L60 light blue; L91 orange, vertically subsampled from the black line). For both ERA-Interim and the operational system, the prior states lie just below the TIL strength scores of the posterior states (blue and red lines) at all latitudes, showing that data assimilation slightly strengthens the TIL globally. However, the degraded observations (light blue and orange) have even better TIL strength scores, meaning that the TIL in both analyses is still weaker than expected from GPS-RO observations degraded to the same vertical resolution (as shown before in Figure 1). Although data assimilation improves the TIL in ERA-Interim and ECMWF (Figures 2 and 3), the TIL there is still weaker and farther away from the tropopause than observed, even if we eliminate vertical resolution as an issue (Figures 1 and 3).

5. Concluding Remarks

Our study is the first to analyze the TIL in the ERA-Interim reanalysis [*Dee et al.*, 2011] at full vertical resolution, directly from its hybrid model levels, the first to show how the TIL is represented in a newer version of the assimilating model (the 2010 ECMWF operational weather forecast system), and the first to describe how the TIL is improved by data assimilation. We summarize our results as follows:

1. Our main finding is that the 4D-Var data assimilation system strengthens the TIL in both ERA-Interim and ECMWF operational systems, as seen in globally positive mean N^2 increments in the TIL region (Figure 2). Therefore, our study updates the findings of *Birner et al.* [2006], who found a weaker TIL in analyses relative to free-running models.
2. To the above, we add that although data assimilation improves the representation of the TIL, it does not completely compensate a common issue in atmospheric general circulation models where the TIL is too far away from the tropopause and generally weaker than expected from GPS-RO observations of the same vertical resolution [*Gettelman et al.*, 2010; *Hegglin et al.*, 2010] (Figures 1 and 3).
3. Both ERA-Interim and a newer version of the same model and assimilation system (ECMWF operational), although having different horizontal/vertical resolutions, show the same structures in terms of N^2 difference from degraded observations, also the same structures of N^2 increments from data assimilation, and both lead to the same conclusions only varying slightly in magnitude. This means that the effect of data assimilation on the TIL remains qualitatively the same when two versions of the same assimilating model with different horizontal/vertical resolutions are compared, suggesting that other factors are of more importance (the model itself, the assimilation technique, and the data sets assimilated). Further experiments would need to be carried out to discern which factors are key.

Our study was conducted for January 2010. Although it is only 1 month, our results show consistent and systematic structures (see sections 3 and 4) across all latitudes in two assimilation systems, indicating their robustness. We showed how data assimilation affects the TIL by analyzing the 4D-Var increments directly. Data assimilation can also improve the representation of dynamics with larger timescale than the assimilation step, like eddies or the residual circulation, and thereby improve the representation of the TIL in the model. A follow-on study regarding this subject is in preparation.

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