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Interactive comment on "Representing the effects of stratosphere-troposphere exchange on 3D O_3 distributions in chemistry transport models using a potential vorticity based parameterization" *by* Jia Xing et al.

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[Comment]: The authors derive an empirical correlation between stratospheric ozone and potential vorticity from two sets of data, with PV from the 21-year WRF simulation and ozone from WOUDC radiosondes during the same period. Specifically, they fit the ratio of ozone to PV as an order-5 polynomial function of latitude and an order-2 polynomial function of pressure (height). The temporal fitting, representing the seasonal variation, is done using a sine function with adjustable amplitude and phase. The spatial fitting is applied to the annually averaged data, so that the fitted model is given by a separable function of time and space. The applicable vertical domain is from 50-100 hPa. The parameterization is then applied to the WRF model to obtain the stratospheric ozone concentration that couples to the air quality model (CMAQ) for year-2006 simulation. The authors give two reasons why they did this study: (1) there is no stratospheric chemistry scheme available in the regional model (2) there is a wide range of measured O3/PV ratio values. The putative success of this parameterization is shown in the one-year simulation (Sim-new) where the results are compared to a reference simulation(Sim-ref) where O3/PV is simply set to be 20ppb/PVU.

[Response]: We thank the referee for the thoughtful and detailed review of our manuscript. Incorporation of the reviewer's suggestions has led to a much improved manuscript. Below we provide a point-by-point response to the reviewer's comments and summarize the changes that have been incorporated in the revised manuscript.

[Comment]: My overall impression is that the authors didn't give much thought in formulating their parameterization (as I explain below). Nor did the authors try to articulate clearly why fitting polynomial functions of higher orders will be better than using the linear correlation in the context of what we already know about stratospheric dynamics and mixing, the photochemical source/sink of ozone and the processes that lead to non-conservation of PV. In my view, if the authors reviewed the stratospheric mixing literature, they could have designed better parameterization and experiments.

[Response]: We agree with the reviewer that as with most parameterizations, the development of a generalized functional relationship between O3 and PV can be further improved. In specific, the function could be better if source and sink of O3 involved in the stratospheric dynamics had been considered in the formulation of the function. However, the design of such a function would require an extensive effort to make the function comply with or redesign the current physics and chemistry structure in the model. It should be noted that most tropospheric chemistry-transport models do not include a representation of stratospheric chemistry in part because the vertical extent (and the resolution employed in the UT/LS) is often limited and also because typical integration time periods are inadequate to represent stratospheric chemistry impacts. The primary motivation of this study is thus to investigate the development of a practical approach to represent the potential impacts of stratosphere-troposphere exchange processes on tropospheric 3D O3 distributions. Unlike most previous tropospheric CTM-based studies that have specified O3 with a fixed scaling factor, here we have attempted to develop a more generalized functional relationship that can capture the seasonal and latitudinal variations in the O3-PV correlation, especially at the higher latitudes. To our knowledge, there are no available functional relationships that can be used for this purpose. We do acknowledge that the current parameterization has some limitation and can be further improved – see for instance the revisions incorporated in response to Referee #1 comments related to representation of UT/LS O3 in the tropics. Additionally, we feel that the suitability, evolution and performance of any parameterization should also consider practical aspects such as the model vertical grid resolution, especially in the UT/LS.

To address the reviewer's concern, we have modified the discussion in the revised manuscript as below:

(Page 7 Line 15-17) "Further improvements to the parameterization should be explored through more detailed analysis of mixing process in the UTLS, through more detailed investigation of the impact of stratospheric chemistry, and improvements in the performance of the parameterizations for conditions representative of the tropical UTLS."

[Comment]: If the authors want to make the case that this is a simple paper based on "big data" statistical approach where the data are trained to relate one variable (PV) to another (ozone) by fitting polynomial functions with no need to discuss the underlying physics and atmospheric dynamics, the authors are then compelled to work out the uncertainty range of the coefficients in Table 1. Is the 20-year data long enough to obtain stable coefficients? If the data are split into two 10-year periods, are the coefficients very different from each other and if implemented in the simulation, would the results be very different from those in the 20-year run?

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[Response]: It is important to note that in developing the O3-PV relationship in this study, we attempted to use all possible available data. Thus we leveraged the existence of a 21-year simulated record of PV in the UTLS with corresponding O3 observations. The relationship developed can thus be considered to be "climatologically" representative rather than representing a specific time period or location. No particular year is used as a training data set. The choice of 2006 for model evaluation was simply based on the fact that this calendar year is also being used for many other assessments with the hemispheric CMAQ because of the availability of additional field campaign data sets (e.g., INTEX-B, IONS, TEXAQS). The good performance with the 2006 upper air observation in fact helps build greater confidence in applicability of the climatological O3-PV relationship. We have recently also completed simulations for the year 2010 and initial analysis suggest similar performance improvements.

Nevertheless, the reviewer raises a good point on the sensitivity of our methodology (and the derived coefficients in the proposed functions) to the length of the data record used. To further investigate the reviewer's question, we split the data into two 10-year periods, i.e., 1990-2000, and 2000-2010. As seen in Figure S8 (Figure C1), the differences between the coefficients derived using different data sets are relatively small. The functions based on data from 1990-2000 and 2000-2010 look quite similar to each other and both are similar to the one based on 21year period used in this study. Further to illustrate that the parameterization is not "trained" for a specific year, we leave out data for the year 2006, and used the remaining 20 years data to parameterize the function. The 2006-leave-out function looks very close to the full-21-years function, and the discrepancy between all coefficients is less than 20%. Therefore, the function parameterized in this study is not specific to a time or location, but rather designed to capture the average variability represented in the long-term record. This information is now included in the revised supplemental information material accompanying the revised manuscript.

To address the reviewer's concern, we clarify this point in the revised manuscript as below:

(Page 7 Line 6-15) “It is important to note that we attempted to use all possible available data in developing the O3-PV relationship in this study. Thus we leveraged the existence of a 21-year simulated record of PV in the UTLS with corresponding O3 observations. The relationship developed can thus be considered to be “climatologically” representative rather than representing a specific time period or location. No particular year is used as a training data set. The stability of the function has been examined by leaving out the year of 2006 for parameterization, and results show that the resulting function barely changed due to this perturbation, suggesting the function parameterized in this study is not specific to a time or location, but rather designed to capture the average variability represented in the long-term record. Figure S8 presents a comparison of the O3-PV functions developed using different lengths of data records. As illustrated by the results, the inferred functions are quite similar across these different data sets, thereby providing some confidence in its robustness in representing the seasonal and latitudinal variations in O3-PV.”

[Comment]: I suspect because the parameterization is confined to the region between 50 and 100hPa, for Sim-new, the free tropospheric ozone concentrations are likely biased high, particularly worse in the winter when the tropopause is the lowest. Here is my reasoning. The tropopause height changes seasonally and STE occurs at the tropopause in connection with the lowermost stratosphere. The tropopause over winter mid- and high-latitudes can be as low as 300 hPa. In other words, the parameterization completely missed the lowermost stratosphere (LMS, defined as the volume enclosed by the 380K isentropic surface/or alternatively the 100hPa isobaric surface at the top and the tropopause below) where the isentropic mixing delivers air and ozone mass across the tropopause. In my view, if one feels compelled to parameterize ozone using PV, then the crucial region where this needs to be done well is the LMS region to capture the isentropic mixing. Even we assume that the Brewer-Dobson circulation transports the correct amount of ozone to the LMS when using the authors’ parameterization, and that the model does the correct mixing, one would still expect that the resulting ozone would still be biased high because of the missing midlatitude photochemical ozone loss in the LMS.

[Response]: We agree with the reviewer that indeed a parameterization such as this could be extended to lower levels, but in this initial study we did not since most regional scale models do not have sufficient vertical resolution in the LMS. In fact early sensitivity simulations, clearly showed that model results were sensitive to the vertical resolution employed (see for instance Mathur et al., 2008; available at: https://www.cmascenter.org/conference/2008/agenda.cfm). To specify O3-PV down to 300mb would also require a much finer vertical resolution. Nevertheless, we agree that the reviewer raises a good point that will be investigated in more detail in future studies and in further evolution of this parameterization. It should however be noted that photochemical loss for O3 in the portions of the LMS included in the model's vertical extent, is represented based on the detailed tropospheric chemistry mechanism used in the modeling system.

To clarify this issue, we have provided the following discussion in the revised manuscript as below:

(Page 7 Line 17-21) "A limitation of this study it that the current model setting lacks sufficient vertical resolution in the lowermost stratosphere. To minimize effects of artificial numerical diffusion associated with the current limited vertical resolution employed in the model, we limit the application of the parameterization to between 100-50mb. Future studies with a much finer vertical resolution, especially to adequately capture the seasonal variation in the tropopause height are suggested to further help evolve the O3-PV parameterization and its practical use."

[Comment]: For the reference case (Sim-ref) the specification of 20 ppb/PVU guarantees a large underestimation of stratospheric ozone as well as a large underestimation of ozone fluxes into the troposphere. It is very common in the literature that the tropopause is defined as the surface of PV= 2 PVU or Ozone =100 or 150 ppb of ozone. These isopleths are in close proximity. This is equivalent to 50-75 ppb/PVU near 150 to 300 hPa. Thus this sim-ref specification of 20 ppb/PVU is not only way too low for 50hPa as the authors already mentioned but is just too low in general. Another way to confirm my suspicion is to check the Sim-new's coefficients at zero-order (constant term) in Table 1, which I presume is the leading term. Indeed, they are 62, 151 and 203 ppb/PVU at 95, 76 and 58 hPa, much larger than 20 ppb/PVU, even near 100hPa. Thus the major finding that Sim-new corrects the negative bias of Sim-ref but overcorrects it for the autumn and winter seasons is largely expected (Page 9).

[Response]: Yes, we agree that the 20ppb/PV unit parameterization will underestimate as it does not account for any variations in the O3-PV relationship in space and time. That precisely is the reason why we embarked on developing this parameterization.

[Comment]: It would be also helpful to see more comparisons of vertical profiles in the free troposphere alone between Sim-ref, Sim-new and WOUDC for the mean and variability of ozone. The log10(ozone) in Fig. 5 only gives a rough sense of magnitude dismatch, mainly that Sim-ref is too weak. The authors should zoom in on the free troposphere for more assessment.

[Response]: The comparisons of vertical profiles in the free troposphere between Sim-ref, Sim-new and WOUDC are given in the Figure S6 (Figure C2). The free- tropospheric ozone is significantly underestimated in Sim-ref. The low bias is reduced in the new simulation with O3-PV parameterization, particularly in mid- and high- latitude regions.

We provided the additional plots as the support information in the revised manuscript.

(Page 5 Line 27-30) "The comparison of vertical profiles in the free troposphere between Sim-ref, Sim-new and WOUDC is given in Figure S6. The free- tropospheric ozone is significantly underestimated in Sim-ref. The low bias is reduced in the simulation with the new O3-PV parameterization, particularly in mid- and high- latitude regions."

[Comment]: It is also better to present pressure height in km or pressure in hPa instead of model layers number in Fig. 5. And more efforts are needed for caption descriptions.

[Response]: The Y scale of Figure 5 has been changed to show both "height in km and pressure in mb" as the reviewer suggested. The figure caption has also been modified, as Figure 5 (Figure C3):

[Comment]: Ultimately this paper is about surface ozone. Judged from Table 3, the surface ozone errors seem quite insensitive to the input of stratospheric ozone (Sim-ref vs Simnew). Have the authors looked into the coupling scheme between the free troposphere and the planetary boundary layer in CMAQ? Any other option for representing the boundary-layer turbulence?

[Response]: As illustrated in Table 3 and Figure 8, errors in surface O3 predictions are quite sensitive to the treatment of stratospheric ozone during spring. Compared to available measurements, the new O3-PV parameterization results in much improved model performance statistics for surface O3 during spring. The accurate representation of 3D transport mechanisms in models is critical for accurately representing the impacts of the stratosphere on lower tropospheric and boundary layer ozone – thus representation of transport by both resolved and sub-grid clouds in addition to the PBL scheme is important. The current PBL scheme in CMAQ is based on ACM2 planetary boundary layer (PBL) model (Pleim, 2007a, b). The scheme has been carefully constructed and implemented in both WRF and CMAQ to maintain consistency in the representation of mixing for both meteorological parameters as well as chemical species. It's been tested and applied in many previous studies and evaluated through comparisons with measurements of vertical profiles of various parameters. However, as suggested by the reviewer, it may be interesting to explore the use of a different PBL scheme in WRF (and CMAQ) model and will be explored in future studies.

Reference:

Pleim, J. E.: A Combined Local and Nonlocal Closure Model for the Atmospheric Boundary Layer. Part I: Model Description and Testing, J. Appl. Meteorol. Clim., 46, 1383–1395, doi:10.1175/JAM2539.1, 2007a.

Pleim, J. E.: A Combined Local and Nonlocal Closure Model for the Atmospheric Boundary Layer. Part II: Application and Evaluation in a Mesoscale Meteorological Model, J. Appl. Meteorol. Clim., 46, 1396–1409, doi:10.1175/JAM2534.1, 2007b.

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Interactive comment

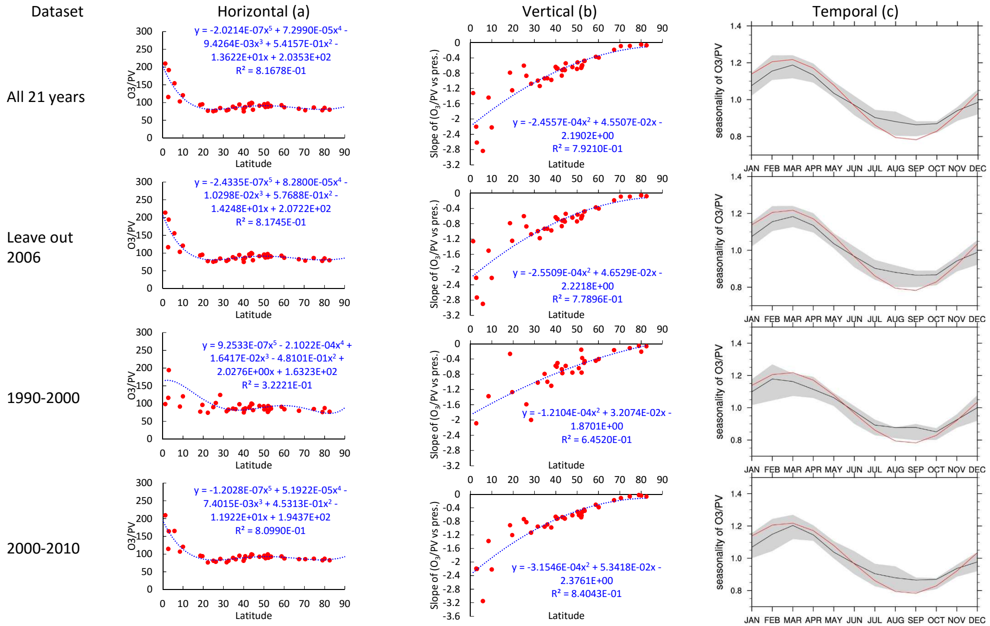

Fig. 1. Sensitivity analysis for the PV function

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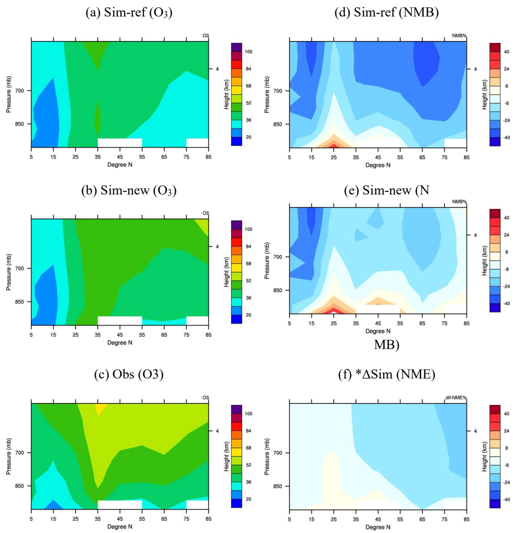

Figure S6. Zonal mean profiles of ozone and error metrics for the different cases in free troposphere (pressure>500mb). (a) Simulated ozone profile in reference case; (b) Simulated ozone profile in new case with updated O_3-PV parameterization ; (c) Observed ozone profile, the annual mean of measurement time period for each WOUDC site across the northern hemisphere; (d) Normalized Mean Bias in the reference simulation; (e) Normalized Mean Bias in the new simulation with updated O_3-PV parameterization; (d) Difference in Normalized Mean Errors between the new simulation and reference simulation (unit: ppb, 2006 Jan-Dec; NMB-Normalized Mean Bias; NME-Normalized Mean Error; *ΔSim= Sim-new minus Sim-ref in NME)

Fig. 2.

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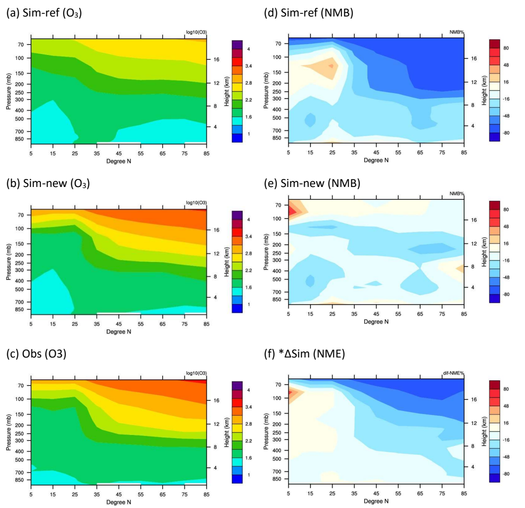

Figure 5: Zonal mean profiles of ozone and error metrics for the different cases. (a) Simulated ozone profile in reference case; (b) Simulated ozone profile in new case with updated O_3-PV parameterization ; (c) Observed ozone profile, the annual mean of measurement time period for each WOUDC site across the northern hemisphere; (d) Normalized Mean Bias in the reference simulation; (e) Normalized Mean Bias in the new simulation with updated O_3-PV parameterization; (d) Difference in Normalized Mean Errors between the new simulation and reference simulation (unit: ppb, 2006 Jan-Dec; NMB- Normalized Mean Bias; NME-Normalized Mean Error; *ΔSim= Sim-new minus Sim-ref in NME)

Fig. 3.