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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We thank the reviewer for the detailed and thoughtful review of our manuscript. Incorporation of the reviewer's suggestion has led to an improved manuscript. Detailed below is our response to the issues raised by the reviewer. We also detail the specific changes incorporated in the revised manuscript in response to the reviewer's comments.

[Comment]: The manuscript introduces a new parameterization for representing vertical, latitudinal, and seasonal variations in upper tropospheric/lower stratosphere (UT/LS) ozone within regional air quality modeling systems. The parameterization is based on regressions between modeled potential vorticity (PV) and observed ozone profiles. Observed ozone is based on measurements from 44 northern hemisphere World Ozone and Ultraviolet Radiation Data Centre (WOUDC) sites. The modeled PV is based on a 21 year (1990-2010) coupled Weather Research and Forecasting (WRF) Community Multi-scale Air Quality (CMAQ) model. The new parameterization is able to account for the significant spatial and temporal variation in $O_3$/PV ratios above 100 hPa and thus provides a much more generalized approach then used in previous studies. The impact of the new parameterization is evaluated by comparing a set of 1 year (2006) WRF-CMAQ simulations with WOUDC and surface measurements. Results show that the new parameterization significantly reduces low biases in the UT/LS compared to simulations with a fixed $O_3$/PV ratio of 20 ppb/PVau resulting in positive impacts at the surface in spring. However, the new parameterization increased the high bias in surface ozone during autumn, resulting in negative impacts during this period. The methodology for developing the new parameterization, results, and conclusions are clearly presented and the work is highly relevant to the air quality modeling community. Figures and Tables in the main body of the manuscript are appropriate as are the supplemental figures.

[Response]: We thank the reviewer for the overall positive assessment of the manuscript and recognition of the implications of the results of the analysis presented.

[Comment]: The $O_3$/PV parameterization relies on the assumption that both $O_3$ and PV are conserved on planetary and synoptic transport time-scales, which is appropriate at middle and high latitudes of the UT/LS. However, in the tropics, sub-grid-scale convective transport largely determines the vertical distribution of ozone while differential diabatic heating due to convective latent heating/cooling introduces a source of UT/LS PV. As a result, the slope of $O_3$/PV verses pressure shows a great deal of scatter for latitudes less than 30N (Figure S2 in the manuscript). This introduces significant uncertainties in the $O_3$/PV regression in the tropical UT/LS and needs to be...
acknowledged. As a result, the new parameterization leads to increased Normalized Mean Errors (NME) compared to the reference simulation in the tropical UT/LS (Figure 5f in the manuscript). A discussion of the appropriateness of using the new O3/PV parameterization in the tropics needs to be included in the manuscript.

(Response): We agree with the reviewer that in the tropics, convective transport plays a significant role in shaping the vertical ozone profile which cannot be fully represented by the UTLS PV. The uncertainties in the O3-PV regression in the tropical UTLS as pointed by the reviewer is also suggested by the poor correlation between O3 and PV at latitudes south of 30N (Figure S2), resulting in an increased NME in Sim-ref in the tropical UTLS (Figure 5f). We agree with the reviewer that this aspect should be further elaborated in the discussions. Following the reviewer’s suggestion, in revised manuscript, we provided additional discussion of the appropriateness of using the new O3/PV parameterization in the tropics, as below:

(Page 3 Line 31-33) “Poor correlation between O3 and PV is found for latitudes south of 30N (Figure S2). This is in part because in the tropics, convective transport plays a significant role in shaping the vertical ozone profile. Consequently, PV alone may not be able to robustly represent UT/LS O3 in the tropics.”

(Page 5 Line 26-27) “An increased NME in Sim-ref is found in the tropical UT/LS, indicating the uncertainty in applying the new O3/PV parameterization in the tropics.”

(Comment): Figure 5 (d) in the manuscript shows that the reference simulation Normalized Mean Bias (NMB) exhibits the classic “C” shaped signature of convective transport and suggests that overestimates in low-level ozone lead to overestimates in tropical UT/LS ozone mixing ratios in the reference simulation. This should be discussed as well.

(Response): We agree that the overestimates in both low-level and UT/LS ozone mixing ratios indicates the influence of the convective transport in the tropics. At the reviewer’s suggestion, we provided additional discussion in the revised manuscript, as below:

(Page 5 Line 21-24) “The overestimates in both low-level and UTLS ozone mixing ratios exhibited in the C-shaped signature in the NMB in Sim-ref is also indicative of the likely influence of convective transport on three-dimensional O3 distributions in the tropics (e.g., Doherty et al., 2005), that is not adequately captured by the current parameterization.”


(Comment): Page 1 line 13: The PV based function does not result in assimilation of UT/LS O3 within WRF-CMAQ. I suggest changing “numerically assimilate” to “parameterize”.

(Response): The “numerically assimilate” has been changed to “parameterize” in the revised manuscript.

(Comment): Page 1 line 14: Change “parameterized” to “developed”.

(Response): The “parameterized” has been changed to “developed” in the revised manuscript.

(Comment): Page 1 line 20: Change “new function” to “new parameterization”

(Response): The “new function” has been changed to “new parameterization” in the revised manuscript.

(Comment): Page 1 line 22: Change “new function” to “new parameterization”

(Response): The “new function” has been changed to “new parameterization” in the revised manuscript.

(Comment): Page 2 lines 10-26: Suggest adding a statement that co-variances between O3 and other species are not accounted for, which might introduce some incon-
sistencies in the chemistry

[Response]: The statement as suggested by the reviewer has been added in the revised manuscript as below:

(Page 2 Line 25-27) “One thing should be noted that such PV based parameterization only modifies the O3 mixing ratio, however, co-variances between O3 and other species are not accounted for in such modifications which might introduce some inconsistencies in the chemistry in the model’s UTLS.”

[Comment]: Page 2 line24: Change “numerically assimilate” to “parameterize”

[Response]: The “numerically assimilate” has been changed to “parameterize” in the revised manuscript.

[Comment]: Page 2 line 25: Change “parameterization” to “development”

[Response]: The “parameterization” has been changed to “development” in the revised manuscript.

[Comment]: Page 2 line 33: Add comment on how many vertical levels are above 100hPa

[Response]: The information of vertical levels is added in the revised manuscript as below:

(Page 2 Line 36-37) “44 vertical layers of variable thickness between the surface and 50 hPa (approximately 3 vertical levels above 100hPa)”

[Comment]: Page 3 line 35: Please comment on the overestimate in the amplitude of the seasonal cycle.

[Response]: The discrepancy in the amplitude of the seasonal cycle between the parametrization and the observations arises due to the difference in the number of sites these curves are representative of. The observed curve was based on data from all sites, while the parameterized curve (red) utilized information only from locations north of 40N. We chose to base the seasonal variations only at sites >40N because that is where the seasonal variability was the strongest. We however agree that this is likely to cause some confusion. Thus we have revised figure 3 (see Figure C1) to now also include observed seasonality based on both (i) all sites, and (ii) sites at latitudes north of 40N.

We clarify it in the revised manuscript as below:

(Page 4 Line 2-6) “The seasonal variability in the O3-PV correlation also varies with latitude. The influence of convective transport on PV in the tropics, as discussed before, also results in weaker seasonal variations in the O3-PV correlation at low latitudes. This is seen in Figure 3, which compares the seasonal variations in this relationship inferred from (i) all sites, and (ii) sites at latitudes north of 40N. Thus to ensure that the parameterization more faithfully captures the seasonality at the higher latitudes, where it is strongest, we parameterize the temporal variations only on data at locations with latitudes north of 40N.”

[Comment]: Page 3 lines 36-38: How well does the new parameterization handle LS ozone loss during Arctic springtime?

[Response]: Basically, the new parameterization is based on long-term observations, thus is able to capture the LS ozone loss which is reflected in the observation. We examined the arctic ozone trend over the past two decades and generally the new parameterization displays good performance in capturing the ozone level and its seasonal variability, as shown in Figure C2. However, it might not be able to capture the potential trend driven by factors other than PV, such as chemistry.

We have clarified this issue in the revised manuscript, as below:

(Page 4 Line 8-11) “Additionally, since only the O3-PV correlation is considered in the parameterization, the potential trend driven by factors other than PV (e.g., chemistry)
cannot be captured by the current parameterization. However, the effects of processes which are already reflected in the observation (e.g., seasonal variations such as lower stratosphere ozone loss during Spring) are implicitly captured in the parameterization.”

[Comment]: Page 5 lines 7-12: Please comment on the role of convective transport coupling the UT/LS and lower level overestimates (see specific comments)

[Response]: The discussion of the role of convective transport to explain the overestimates of UT/LS and lower level O3 has been added in the revised manuscript, as below:

(Page 5 Line 21-24) “The overestimates in both low-level and UTLS ozone mixing ratios exhibited in the C-shaped signature in the NMB in Sim-ref is also indicative of the likely influence of convective transport on three-dimensional O3 distributions in the tropics (e.g., Doherty et al., 2005), that is not adequately captured by the current parameterization.”

Reference:

[Comment]: Figure 4: Sim-new maps should be the same size as the WOUDC and Sim-ref maps.

[Response]: We adjusted the size of Sim-new maps to be the same size as the other two in the revised manuscript.

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Fig. 1. Seasonality of O3/PV (Annual mean= 1, black solid line= observed mean at all sites, grey, black dash line= observed mean at sites at latitudes north of 40N, red line = fitted by function)
Fig. 2. O3 trend in the top layers (pressure<100hPa) in the Arctic (latitude>75N)