

Interactive comment on “Representing the effects of stratosphere-troposphere exchange on 3D O₃ distributions in chemistry transport models using a potential vorticity based parameterization” by Jia Xing et al.

Anonymous Referee #2

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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

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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.

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.

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?

I suspect because the parameterization is confined to the region between 50 and 100 hPa, 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 com-

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pletely 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.

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).

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 $\log_{10}(\text{ozone})$ in Fig. 5 only gives a rough sense of magnitude mismatch, mainly that Sim-ref is too weak. The authors should zoom in on the free troposphere for more assessment. 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

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descriptions.

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 Sim-new). 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?

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