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Interactive comment on "Comparison of Chemical Lateral Boundary Conditions for Air Quality Predictions over the Contiguous United States during Intrusion Events" *by* Youhua Tang et al.

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Thank you for your review. We made comprehensive revisions according to your suggestion. The figures 13/14 were re-plotted and added another run for summer 2018 case. Here are the answers to your comments

Review of Tang et al. "Comparison of Chemical Lateral Boundary Conditions for Air Quality Predictions over the Contiguous United States during Intrusion Events" In this paper, Tang et al., use a number of different methods to set boundary conditions for use in CMAQ as part of the US NOAAs forecasting system. While focusing on PM2.5, they also looked at ozone. Not surprisingly, they found that having boundary condi-

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tions that are more representative of actual conditions improved model performance. The manuscript needs to be thoroughly edited for grammar before resubmission. It is replete with incorrect inclusion or exclusion of articles (in the grammatical sense).

âĂć Thank you for your comments. We follow your suggestions to make the literature revision and correct the gramma issues. Please see below for the details.

They also inconsistently used plurals and singulars, including when the used the terms LBC(s) and CLBC(s). Given that you typically set more than one boundary condition, it should almost always be plural, but either way, be consistent. They tend to use ambiguous ronouns (e.g., its).

âĂć Great suggestion. We made changes to be consistent. The LBC(s) and CLBC(s) are used in three circumstances: general term, one LBC vs another LBC, and several LBCs. Now the plural word is used under only the third circumstance.

After fighting through the manuscript, the third sentence of the Conclusion was: “The GEOS dynamic LBC showed the overall best score when comparing with the surface observations during the June-July 2015 while Saharan dust intrusion and Canadian wildfire events occurred.” “LBC” should be “LBCs”, “comparing”should be “compared”, “the June” should be “June”, “while” should be “when”, ”Saharan” should be “the Saharan” (at least I think those are appropriate).

âĂć Changed

In the Introduction, they state that there are two roles “it” (actually they, i.e., CLBCs) play. The two are the same. They are setting values of the concentrations used in solving the differential equations that underlie the core of an air quality model. In such a way, they might be called constraints, but that is both awkward and imprecise, as they are not setting a range, but an actual value. This is exactly how external influences are brought in to the model. Using the precise definition of boundary condition leads to (1) and (2) being the same.

âĂć You are right that the CLBC has one value, though it can be static or dynamic. Now the sentence is changed to be “The CLBC sets concentration values along the regional domain’s lateral boundary, and those setting values have two effects in the regional modeling system depending on the CLBC types (static or dynamic) and the events.”

Line 14: “Proper” is not the best word here. What defines proper? Do they mean accurate? How accurate?

âĂć You are right that a suitable word is needed here, and “proper” is not the best. We changed it to “certain” since regional model need a lateral boundary condition to run, regardless good or bad LBC.

Line 26: Sentence beginning Tang et al.: What point is being made?

âĂć Changed. We added “For non-intrusion events,”

The description of the 5 model runs should be more clear, with specifics in a Table.

âĂć Changed Table 1 to be clearer.

ACP is an international journal, so the US NOAA should be used at least the first time and NOAA defined.

âĂć Added the definition of NOAA

Page 3 Line 34: : : Not sure what this is adding.

âĂć Changed to “We developed a tool to extract the GEOS-LBC along the NAQFC’s domain boundaries”

The title should be a bit more explanatory as Intrusions can be stratospheric, still impacting lateral boundary conditions.

âĂć Changed to “pollutant intrusion events”. Actually, the two GEOS-LBCs included stratospheric ozone influence (Figure S1) from the GEOS global model, which is the

reason of their better correlations (Table 5). This study focused on influence on surface O3/PM2.5, so the stratospheric intrusion was not strongly highlighted.

Page 10, line 35. The surface stations reflect the wildfire intrusions just as well as VIIRs at their location. The issue here is how well the surface stations provide more spatial coverage.

âĂć Yes, your words are better for what it actually means. We changed. In fact, we first tried to use surface monitoring data as indicators as that in-situ surface data is more reliable and has better temporal resolution (hourly). However, its poor spatial coverage is not good enough for this purpose.

Page 11, line 20: I do not think that “a high pressure system controlled western Canada” (the authors should look at that whole sentence).

âĂć Changed to be Figure S4 showed that there was a high-pressure system with peak surface pressure up to 1022 hPa in the western Canada.

P3 L20-21. Why does the CMAQ_BASE simulation use a clean background for aerosols.

âĂć We added the explanation. The clean background aerosol LBC was used in the operational NAQFC before the NGAC model data was available, since the CONUS domain’s boundaries lay on the ocean or less polluted regions. Switched Figures 1 and 2.

According to the introduction, the NAQFC system currently uses NGAC for its aerosol LBCs? Does this not make the performance of the CMAQ_BASE simulation artificially worse than the current NAQFC system? And if your goal is to compare how new CLBCs impact the forecast, shouldn’t the CMAQ_BASE simulation represent what is used in the current NAQFC system? It is not clear to me if any of the 5 simulations listed in Table 1 use the same CLBCs as the current NAQFC system, though I think it may be NGAC-LBC. This should be clarified.

âĂć It was clarified in the introduction “The current NAQFC uses the dust-only aerosol CLBC from NGAC”. So, current NAQFC just use the dust LBC from NGAC, not the full-GOCART aerosol LBC, as there were some issues in NGAC’s other aerosol prediction, including wildfire. The CMAQ_Base was not artificially worse, and that LBC was actually used in the old NAQFC system before NGAC was available.

Figure 7. There appears to be a discontinuity at the transition between the east and north boundaries. Is this correct, and if so, what could cause this?

âĂć It is correct. CMAQ’s boundary index is always from south to north and from west to east. So the boundary index’s start points are reset instead of continuous for north and west boundaries. You can find the boundary structure in https://www.cmascenter.org/ioapi/documentation/all_versions/html/THKBDY.jpg. We added the explanation in Figure 3’s captions.

If the details of the mapping are important, the chemical mapping is a bit haphazard. Putting all of the MVK in to ISPD would require that all of the MVK comes from isoprene. Splitting all of the INO2 using the coefficients in the ISOP+NO3 reaction would require that all of the species degrade at a similar rate, or that INO2 rapidly reacts to those products.

âĂć Yes, you are right for these issues. GEOS model’s MVK comes from Isoprene and there is no MVK emission. So the MVK mapping to ISPD of CMAQ’s CB05 is consistent with its source in GEOS. For the intermediate INO2, GEOS has this explicit species, and it has the following reactions, such as INO2+MO2 = 0.55NO2 + 0.40HO2 + 0.425HNO3 + 0.025NO2 + 0.05MACR + 0.08CH2O + 0.03MVK + 0.25RCHO + 0.75CH2O + 0.25MOH + 0.25ROH + 0.05HO2. CMAQ’s CB05 mechanism bypasses the intermediate INO2, and assumes ISOP+NO3 directly generate some similar final products. It is true that we can not achieve perfect consistence for these species mapping as these two mechanisms are so different. Fortunately, for the CONUS domain, the isoprene chemistry influence’s on the CONUS LBC is less significant compared to

the major intrusion events of wildfire plume and dust storm as the short-lived isoprene hardly reach farther downwind. I added the explanation.

ALK4 includes C4 and higher alkanes, so having it turned in to 4 PARs is biased low unless it is all butane isomers. A detailed understanding of both mechanisms are needed to do such a mapping directly if this step is important to be done in detail (which I am not sure it is: : : for boundary conditions, the important species are probably NO, NO2, O3, PM species, SO2, NH3, HCHO and a few others, but that is just a guess: they might check that out. Having to deal with large fires may lead to large fluxes of other organics that then become important. They need to work on a better way of expressing their finding that setting better boundary conditions leads to a better simulation.

âĂć Yes, it is true that this treatment could have a "truncation error". However, the GEOS global model itself also treat the ALK4 mainly as butane: ALK4+OH = R4O2, R4O2+NO $\rightarrow$ NO2 + 0.32ACET + 0.19MEK + 0.18MO2 + 0.27HO2 + 0.32ALD2 + 0.13RCHO + 0.50A3O2 + 0.18B3O2 + 0.32ETO2, or Cn with n$\sim$4. For the LBC, the issue of C5 or higher alkanes treatment may only appear if strong C5+ alkane emissions existed outside of our domain and were not too far (penpane's lifetime is around 4.6 days (Helmig et al, 2014 (doi:10.5194/acp-14-1463-2014), and hexane has even short lifetime than butane), and the global model treated the C5+ alkanes emission and reaction more explicitly. For our cases, only big wildfire emission could have this impact in real world, though the wildfire C5+ alkane emission is at least one order of magnitude lower than the corresponding CO/Ethane/Propane emission (Urbanski et al, 2008, DOI:10.1016/S1474-8177(08)00004-1). Also, the GEOS did not treat C5+ alkanes explicitly to capture the real-world situation. So, the C5+ alkane mapping for LBC unlikely make big difference in our simulations with that "truncation error". In fact, the difference between GEOS and CMAQ's carbon bond mechanisms, and the uncertainty of wildfire emissions could be bigger issues, but they are beyond the content of this manuscript. We added some related explanations in the manuscript.

The results from the AOT-derived LBC to be a more compelling idea and would have

liked to see a comparison of CMAQ performance using the AOT-derived LBC and the dynamic LBC (GEOS-LBC and NGAL-LBC), but these were not modeled for the same time period as the AOT-NLBC case. Is the use of three or four significant figures justified?

âĂć Good suggestion. We added the NGAC-LBC for the summer 2018 comparison. Some related discussion and figures are also expanded.

In the end, there are aspects of this paper of potential interest to ACP readers, but at this juncture, the grammar and some of the set up needs work before it should be further considered for publication in ACPD or elsewhere. The authors need to identify and highlight what is unique about their findings other than “better boundary conditions lead to better results.” What is the best approach and why? (or, what are the positives and negatives of each approach and what is a general recommendation after weighing those attributes?) This should be stated concisely in the Abstract and the conclusions, backed up with specific study results.

âĂć Thank you for your encouragement. We revised the conclusions and abstract, and made thorough literature editing through the manuscript. Please see revised manuscript for detail.

Again. Thank you for your comments

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