#### We thank Jonathan Pleim for his detailed comments that helped improve the manuscript.

Reviewer #1:

#### General comments

This study aims to evaluate different techniques involving ingestion of vegetation, soil temperature and moisture, and SST data from satellite and LDAS output, to improve high-resolution WRF simulations for use with the CMAQ air quality model applied to the LMOS field study. The study also includes two different physics configurations that alter the LSM, PBL, and microphysics. Unfortunately, the model configuration designated "EPA" seems flawed relative to our experiences modeling many fine scale domains. How it may be flawed, however, can only be speculated. I think more should be done before this "EPA" simulation is used. We understand that many users may not fully appreciate some of the details in configuring inputs and some namelist settings (i.e., Obsgrid) that need some scale awareness, but we think that a sensitivity study of different physics configurations should make sure the model has the most appropriate inputs and runs correctly. Instead, the paper seems to suggest that these results are just what you get when running the "EPA" configuration. Also, calling what they have done the "EPA" configuration makes it seem like they were either performed by the US EPA or endorsed. The EPA has used similar configurations at high-resolution with good results as shown in the recently published LISTOS modeling study (Torres-Vazquez et al. 2022). The LISTOS area is just as complex as LMOS with land-sea breeze impacts. The LISTOS modeling showed that the 2-m temperature RMSE for the 1.33 km domain were clearly lower than the 12 km (1.75 K for 12 km and 1.60 K for 1.33 for the whole summer) which is also much lower than the LMOS results shown here. The reasons for the poor results may be related to the data assimilation procedures/inputs used in this study. However, it is not clear from the manuscript what was done in some key areas of data preparation.

It is mentioned that the indirect soil moisture and temperature nudging was used in the PX LSM. Some details are not clear. It seems that they used the 0.25-degree resolution GFS Final re-analyses available at 6-h intervals as background to re-analyze with MADIS observations using OBSGRID. However, these analyses are much too coarse spatially and temporally to give good results for WRF runs at 1.33 km resolution which would explain why the results are not as good as the runs used for LISTOS which used the UnRestricted Mesoscale Analysis (URMA) data set, available in as fine as 1-hourly increments on a 2.5 km grid spacing for 1.33 km WRF runs. Some of these ideas for best practices for running the PX LSM at high resolution are described in a document <a href="http://www2.mmm.ucar.edu/wrf/users/docs/PX-ACM.pdf">http://www2.mmm.ucar.edu/wrf/users/docs/PX-ACM.pdf</a> referenced in the WRF users' guide <a href="https://github.com/wrf-model/Users\_Guide">https://github.com/wrf-model/Users\_Guide</a>. However, this alone is unlikely to have resulted in the large errors and biases especially in humidity that are shown in the paper. Therefore, I think there may have been other issues like potentially problems with the observation nudging.

It is stated several places that surface observation nudging was used for the "EPA" runs, but the details of how this was done are not described. On lines 470-472: *The superior performance of the EPA simulation on the 12-km domain is partially an artifact of its use of surface observation nudging because the same observations used in the nudging routine were also used for verification.* If the same observation nudging was used for the 1.33 km runs the results would also show superior

performance at the observation locations. Seems something went wrong and likely an issue with the nudging itself. Until the flaws in the "EPA" runs are investigated, discovered, and corrected, I suggest that these simulations be removed from the study. It seems like the experimental design implicitly linked obs nudging to the US EPA configuration. We think this should have been a separate sensitivity.

The comparisons of the various YNT sensitivity simulations show relatively small differences. There are some interesting analyses of the differences and discussion relating the differences to the variations in the use of soil, vegetation, and SST data sets and a change in the height of analysis FDDA. However, these discussions repeatedly refer to comparisons to the flawed "EPA" runs.

Thank you for your comments. We have changed "EPA" to "AP-XM" throughout the revised manuscript to avoid the appearance that these simulations were performed or endorsed by the EPA. The new naming convention follows that of the "YNT" configuration (e.g., initials for the names of the PBL, LSM, and microphysics schemes). We appreciate your concern about the accuracy of the EPA (AP-XM) simulation. We have confirmed that the namelist options we used for this simulation are correct; however, given the presence of the large moist bias, we cannot rule out that there was a problem with its implementation. Because we are unable to run new simulations at this late stage of the project, we have instead decided to include results from an earlier version of the "EPA" simulation that we had run that did not use observation nudging or soil temperature and soil moisture nudging, which is hereafter referred to as the "AP-XM" simulation. The figure below shows the summary statistics for this simulation along with the old EPA simulation (which is named AP-XM\_OBS in the figure) that used observation and soil nudging. Though the temperature and wind speed errors in the AP-XM simulation (without soil and observation nudging) are slightly larger than the AP-XM\_OBS simulation (with soil and observation nudging), the water vapor bias and RMSE have been greatly reduced. The overall conclusions from this sensitivity test remain the same as before where the AP-XM configuration provides superior results for 2-m temperature and 10-m wind speed on the 12-km domain but then becomes less accurate than the YNT configuration on the 1.3-km resolution domain, while also having a moist bias and larger water vapor RMSEs on all three domains.

Based on this sensitivity test, we have decided to include results from the "AP-XM" simulation without observation and soil nudging in the revised manuscript. This has the notable advantage of allowing us to avoid the situation where the same surface observations used for the evaluation are also used in the observation nudging routine for one of the simulations. This means that the evaluation methods can be applied evenly across all of the model simulations, which strengthens the conclusions of the revised paper. It also eliminates potential biases being introduced though sub-optimal use of the observation and soil nudging schemes. Though the document noted by the reviewer recommends that nudging should be used with the Pleim-Xiu land surface model, the decision not to use it in the AP-XM simulation in this study is supported by the fact that there have been many studies over the past few years that have used the Pleim-Xiu scheme without observation or soil nudging (e.g., Bhautmage et al. 2022, J. Geophys. Res.; Parra 2023, Atmosphere; Parde et al. 2022, Atmos. Res.; Lu et al. 2021, Clim. Dyn.; Jacondino et al. 2021, Energy). Nonetheless, to acknowledge these additional tools, we have added two sentences to the second paragraph in the conclusions section describing results from the AP-XM simulation stating that: "In addition, use of observation nudging and soil moisture and soil temperature nudging as used in Torres-Vazquez et al. (2022) would also help constrain the evolution of this simulation. Though these specialized nudging techniques were not employed in our study due to their added complexity and confounding influence on the model evaluations because the same observations used in the nudging procedure would also be used to assess the accuracy of the simulations, their utility could be assessed in future work."

	Bias				% RMSE Change vs. AP_XM_OBS				% RMSE Change vs. YNT			
	a) 2-m Temperature [K]				b) 2-m Temperature [K]				<b>c)</b> 2-m Temperature [K]			
Simulation	12 km	4 km	1.3 km		12 km	4 km	1.3 km		12 km	4 km	1.3 km	
AP_XM	-0.66	-0.85	-0.14		2.27	2.36	3.03					
AP_XM_OBS	-0.12	-0.40	0.16		2.03	2.23	3.00					
YNT	0.16	0.47	0.55		13.08	0.45	-25.18		2.30	2.24	2.25	
YNT_SST	0.17	0.48	0.56		12.44	-0.13	-25.58		-0.57	-0.58	-0.53	
YNT_SOIL	-0.39	-0.19	-0.22		11.95	-4.62	-30.41		-1.00	-5.04	-6.99	
YNT_N2KM	0.25	0.58	0.67		12.44	-0.18	-24.68		-0.57	-0.62	0.67	
YNT_GVF	-0.28	-0.02	-0.03		12.54	-1.88	-27.91		-0.48	-2.32	-3.65	
YNT_SSNG	-0.56	-0.32	-0.38		10.62	-5.20	-29.71		-2.17	-5.62	-6.06	
YNT_SSN	-0.29	-0.07	-0.09		9.00	-7.44	-31.91		-3.61	-7.85	-8.99	
	d) 2-m Mixing Ratio [g/kg]				e) 2-m Mixing Ratio [g/kg]				f) 2-m Mixing Ratio [g/kg]			
Simulation	12 km	4 km	1.3 km		12 km	4 km	1.3 km		12 km	4 km	1.3 km	
AP_XM	0.38	0.64	0.60		1.67	1.80	1.70					
AP_XM_OBS	0.91	1.28	1.35		1.85	2.03	2.07					
YNT	0.19	0.00	-0.20		-19.96	-28.69	-29.85		1.48	1.44	1.45	
YNT_SST	0.20	0.00	-0.20		-20.66	-29.19	-30.48		-0.88	-0.69	-0.90	
YNT_SOIL	0.24	0.10	-0.02		-20.12	-29.14	-31.40		-0.20	-0.62	-2.21	
YNT_N2KM	0.22	0.05	-0.14		-19.69	-28.10	-28.88		0.34	0.83	1.38	
YNT_GVF	0.30	0.17	0.02		-20.12	-28.69	-30.77		-0.20	0.00	-1.31	
YNT_SSNG	0.36	0.28	0.24		-22.33	-29.83	-31.54		-2.96	-1.59	-2.41	
YNT_SSN	0.27	0.14	0.04		-21.20	-29.83	-32.03		-1.55	-1.59	-3.10	
	g) 10-m Wind Speed [m/s]				h) 10-m Wind Speed [m/s]				i) 10-m Wind Speed [m/s]			
Simulation	12 km	4 km	1.3 km		12 km	4 km	1.3 km		, 12 km	4 km	1.3 km	
AP XM	-0.02	-0.22	-0.23		1.51	1.50	1.62					
AP XM OBS	0.05	-0.17	-0.14		1.52	1.51	1.63					
YNT	0.45	0.34	0.36		6.26	2.19	-3.32		1.61	1.54	1.57	
YNT SST	0.46	0.34	0.36		6.52	2.52	-2.40		0.25	0.32	0.95	
YNT SOIL	0.38	0.24	0.23		5.07	1.26	-4.49		-1.12	-0.91	-1.21	
YNT N2KM	0.42	0.32	0.34		4.61	0.60	-5.05		-1.55	-1.56	-1.78	
YNT GVF	0.60	0.54	0.60		10.87	7.97	4.06		4.34	5.65	7.64	
YNT SSNG	0.53	0.47	0.49		8.04	5.25	-0.25		1.67	2.99	3.18	
YNT_SSN	0.36	0.23	0.22		3.82	-0.20	-6.52		-2.29	-2.34	-3.31	
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Specific comments:

Line 20: Please do not refer to the simulation using PX and ACM2 as "EPA" since the EPA was not involved with these runs.

## We have changed "EPA" to "AP-XM" here and elsewhere in the manuscript.

Line 24: "physically unrealistic ground heat flux". This should have been a clue that something was seriously wrong and should be investigated.

Prior to submission of this paper, we verified that we had used the correct settings and run-time options for the "AP-XM" (nee EPA) simulation. We cannot rule out that there could be a bug in the version of the P-X LSM available in version 3.8.1 of the WRF model, but the fact that the ground heat flux has a realistic diurnal pattern and the other surface fluxes are very similar to those of the YNT simulations on the 12-km domain but then becomes unrealistic on the 1.3-km domain points toward limitations in the AP-XM configuration when used at higher resolutions.

Line 93: This is a 7 year old version of WRF. Why not use a newer version? There have been significant changes and error corrections in PX and ACM2 since then. Noah has also been updated.

This project began in late 2018. The version of the WRF model that we used during this study was just over a year old at the start of the project. To maintain consistency, we decided to keep using that version of the model throughout the project. We were planning to submit this paper during 2020 but then decided to wait until we could submit it along with our evaluation of the CMAQ model simulations (part II of this study). That decision, along with delays due to covid, meant that we did not submit this paper until earlier this year.

Line 111: misleading. Better to say local and non-local vertical transport

## This sentence has been revised as requested.

116: "available surface observations" is not 100% accurate here. The indirect nudging uses the surface analysis in the wrfsfdda\_d0\* files. Obsgrid creates the wrfsfdda\_d01 file using the GFS-FNL here + MADIS point obs, but it is more accurate to say the indirect soil nudging uses a surface analysis from Obsgrid.

## This sentence has been removed because we are no longer using observation nudging.

121-123: More explanation is needed especially about the background analysis

## This sentence has been removed from the revised manuscript because we are no longer using observation nudging in the AP-XM simulation.

144: If I understood correctly some of these datasets are use daily not just for initialization

Thank you for the comment. We have decided to refer to these as "surface datasets" rather than "surface initialization datasets" because, as you point out, they are used not only to initialize the model but also to update the surface fields each day. Revisions have been made throughout the manuscript to account for this change.

Table 1. Please clarify what is meant by "obs nudging to MADIS". Is this direct obs nudging or the indirect soil T and SM nudging using obsgrid?

## This statement has been removed because we are no longer using observation nudging in the AP-XM simulation.

231-233: Again, need to explain surface nudging

## This sentence has been removed because we are no longer using observation nudging in the AP-XM simulation.

270-272: Basic rule of thumb: don't use coarser analyses to nudge finer models

This sentence has been deleted from the revised manuscript because we are no longer using observation nudging with the AP-XM simulation.

283-284: This is unreasonable performance. The simulation should be fixed or removed from comparison.

We have replaced the EPA simulation with the AP-XM simulation that does not use observation or soil nudging. For 2-m temperature, the AP-XM simulation provides superior performance on the 12-km domain and comparable performance on the 4-km domain, but was less accurate on the 1.3-km domain when compared to the YNT simulations.

310-311: This suggests deficiencies in YNT physics

We have added this sentence to the end of this paragraph: "This behavior could also be due to deficiencies in the YNT configuration over complex urban-lake transition zones."

334: The fact that WS errors were smaller for "EPA" than T2m and q-2m suggests that the data used for soil nudging was very detrimental.

We state in the second paragraph of Section 3.1 in the revised manuscript that the AP-XM run contains the smallest wind speed bias on all three domains and lower RMSE on the outermost two domains when compared to the YNT simulations.

362-365: This shows some serious errors in the "EPA" runs. Need to figure that out or remove from comparisons.

# We have replaced the EPA simulation with the AP-XM simulation that does not use observation nudging or soil nudging. The water vapor errors are much smaller now, though the temperature and wind speed errors are similar to what was obtained during the EPA simulation.

405: This assumed surface energy balance neglects Cp dTg/dt. Why not sum the up and down SW and LW components? That would be net surface radiation.

## Thank you for the suggestion. We have revised Fig. 7b so that the net radiation is now computed using the sum of the upward and downward shortwave and longwave radiation components.

425-434: These results seem to indicate that there is a larger problem than the low resolution of the nudging data. The Gflux always < 0 and the large wet bias day and night suggests that the nudging data is much too cold. If a DA scheme uses bad data, the results will be bad. The surface nudging analyses should be evaluated the same way as the model output. I expect this will show large errors in the nudging data. This might suggest errors in the OBSGRID processing.

The revised manuscript includes results from the AP-XM simulation that did not use observation or soil nudging. The overall pattern remains the same to what was found in the original "EPA" simulation that used observation and soil nudging, namely that the diurnal cycle of the ground heat flux was similar to the YNT simulations on the 12-km domain but was consistently negative on the 1.3 km domain. This points toward this behavior not being due to the coarse resolution of the nudging data.

445: This is contrary to what the LISTOS study showed

## This sentence referred to the behavior of the surface flux terms during the AP-XM simulation. Torres-Vazquez et al. (2022) did not evaluate the accuracy of these terms in their paper.

460: Again, please clarify "surface observation nudging"

### Surface observation nudging is no longer used during the AP-XM simulation.

462: Noah is not more sophisticated than PX LSM overall. While Noah has more soil layers, PX uses more refined representation of land use related parameters. Also, the indirect soil nudging capability is a big advantage when applied correctly as has been demonstrated many times in many publications. In other ways the two models are roughly equivalent.

### This sentence has been removed from the revised manuscript.

464: Again, not just initialization.

# As mentioned earlier, we now refer to these datasets as "surface datasets" rather than "surface initialization datasets" because, as you point out, they are used not only to initialize the model but also to update the surface fields each day.

470-472: if the good performance of the 12 km "EPA" run is due to obs nudging then why did the 1.33 km run not have similarly good results. Observation nudging using the same obs as used in the statistics should give much, much better results.

The revised manuscript includes results from the AP-XM run that does not employ observation nudging. With this new run, there is still a moist bias on all three domains, but it is much smaller than occurred when using observation nudging.

474-476: I agree that the relative spatial sparseness of the obs do not accurately capture and constrain small-scale features on the 1.33 km grid but evaluating with the same observations as used on the obs nudging should result is very close agreement regardless of the model grid scale. This suggest some potential problem with the obs nudging that should be investigated, or removing Obs nudging from the experiment or as an independent sensitivity

# The revised manuscript includes results from the AP-XM run that does not employ observation nudging.

485-488: The two-layer soil structure is designed to work with the indirect nudging. This normally works well and gives better results that other LSMs when applied correctly.

We have added two sentences to the end of this paragraph noting that: "In addition, use of observation nudging and soil moisture and soil temperature nudging as used in Torres-Vazquez et al. (2022) would also help constrain the evolution of this simulation. Though these specialized nudging techniques were not employed in our study due to their added complexity and confounding influence on the model evaluations because the same observations used in the nudging procedure would also be used to assess the accuracy of the simulations, their utility could be assessed in future work."