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Geoscientific Model Development Discussions

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Interactive Comment

Interactive comment on "Turbulent transport, emissions, and the role of compensating errors in chemical transport models" *by* P. A. Makar et al.

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General Comments:

This study addresses a long standing dilemma in air quality modeling involving lower limits for eddy diffusivities in chemical transport models (CTM). Historically, most air quality models used rather large values for minimum eddy diffusivities (e.g. 0.5 – 2.0 m2/s) to avoid gross over predictions of primary emitted species during nighttime. A side effect of this practice was over predictions of nighttime ozone because of too little NO titration. This seemed to be a reasonable strategy since it resulted in better evaluation of PM2.5 for which the relevant standards are 24 hour averages without compromising the daytime ozone evaluations for which the standard is 8-hr maximum concentration (in the US). The downside of this idea is that it is fundamentally incorrect

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since there is no physical justification for using eddy diffusivities in the CTM that differ from those used in the meteorology model. Meteorology models typically have very low eddy diffusivity minimum values (e.g. 0.01 m2/s) for numerical considerations. Using values that are greater than the eddy diffusivity values computed by the PBL schemes during stable conditions is unjustified. Thus it is reasonable to conclude that if air quality models produce better results with the greater minimum eddy diffusivity values then it is compensating for other errors. While it is clear that this is the main thesis of this paper, the point that the greater minimum eddy diffusivity values used in some models, typically older models, is scientifically unjustifiable should be made more strongly from the start. I think this point has been recently recognized in the modeling community resulting in the reduction in these artificially high minimum values. This historical and evolving perspective should be clearly presented.

An example of this progression away from artificially high minimum eddy diffusivities is in the changes to the CMAQ model in recent years. The version used in this study was released in 2006 and is therefore significantly out of date. In that version of CMAQ and earlier versions the minimum eddy diffusivity was set to 1.0 m2/s everywhere. Soon after that, CMAQ was revised to use 0.5 m2/s in rural areas with a ramp up to 2.0 m2/s in urban areas with the recognition that the model was not capable of accounting for the turbulence enhancing effects of urban environments. More recently, with the release of CMAQv5.0 (2011) and v5.0.1 (2012) the minimum eddy diffusivity used in CMAQ is 0.01 m2/s for rural areas, which is identical to the minimum used in the ACM2 PBL scheme in WRF, and 1.0 m2/s in urban regions. Note that the urban value is weighted by the area fraction of urban land use in each grid cell which is a very small fraction of the total area in most modeling domains. Thus, I don't think that it's acceptable to use CMAQv4.6 in this study since a main object of the study, the minimum eddy diffusivity, has been drastically revised since then. Also, there have been many other upgrades to CMAQ since v4.6 that could affect the evaluation and model comparison results. It is clearly not representative of the comparative performance of the two models to use such an outdated version of CMAQ compared to a more recently updated version

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of AURAMS. The sensitivity of model results to the magnitude of the minimum eddy diffusivity is sufficiently demonstrated through the comparison of the AURAMS scenarios, particularly AURAMS5 where the minimum eddy diffusivity is set to 0.6 m2/s. The comparison to CMAQ seems to be superfluous to the main objectives of the paper. I suggest the CMAQ part either be removed or the CMAQ results be replaced with runs using CMAQv5.0.1, which is publically available at www.cmascenter.org.

The main point of the paper that the nocturnal overpredictions of PM2.5 when lower values of eddy diffusivity are used are largely attributable to the diurnal allocation of emissions seems too simplistic. While the models are clearly sensitive to this as shown in this study, there may be many other factors contributing to these concentration errors. Most of the emission modifications seem to be corrections that should be made anyway. The final test (AURAMS6) represents an extreme and unrealistic sensitivity test which does show that the model is sensitive to the diurnal emission profiles, reducing the nocturnal high bias in PM2.5 but increasing the frequent daytime high bias.

In the introduction section there is an extensive review of previous model comparison and evaluation studies. The results of the AQMEII study are particularly well described including model performance of not only PM2.5 and PM10 but also particular speciated aerosols such as seasalt, organic, and inorganic and processes like dry deposition and stable boundary layers. In contrast, the present study seems too limited as is admitted in the discussion section. The focus is totally on minimum eddy diffusivity and emission diurnal temporal allocation. Also, the evaluation is exclusively on ozone and PM2.5 whereas analysis of model performance for primary versus secondary PM and primary gasses such as CO and NOx would probably enhance understanding of model and emission errors.

Specific Comments:

P5598 ln21: I think “consistently matched” needs some elaboration.

P5600 lns19-25: The CMAQ version is quite out of date (7 years old) while the AU-

RAMS has been recently updated. Is the AURAMS1b scenario the updates describe in Kelly et al (2012)? If so, please summarize what these updates entail.

P5601 ln10-11 and ln23: The meteorology data is interpolated to a 12 km grid for the air quality modeling but the type of map projection is not mentioned.

P5602 ln11-14: This short paragraph is the entire description of the dry deposition calculations of the 2 models. Considering the importance of dry deposition to the concentrations of gasses and aerosols as demonstrated in the AQMEII study, I think there should be much more description, comparisons, and sensitivity model runs included. The reference given for the CMAQ dry deposition is actually a description of the implementation and testing of the Pleim-Xiu land surface model (PX LSM) in the MM4 and not about dry deposition. CMAQ is usually run with WRF using the PX LSM so that the stomatal conductance and aerodynamic conductance as well as land use related parameters such as roughness length, LAI, vegetation fraction, etc, can be read directly from the WRF output and used in CMAQ for calculating dry deposition velocities. Since this study uses GEM for meteorology, the dry deposition calculations cannot follow this usual procedure and therefore should be described here.

P5604 ln12-13: To make the model evaluations more comparable, the hourly average output from CMAQ (ACONC output file) could be used with the AURAMS hourly averages.

P5605 ln 9: Perhaps this is a good place to explain what updates went into AURAMS1b. Section 4.2.5 could be moved to this location.

P5606 ln1: Calling these results a "marked difference" from the earlier study (Smythe et al. 2009), seems to be an overstatement. Both studies showed that "AURAMS outperformed CMAQ" for most statistical metrics. The bigger differences seem to be with the even earlier studies (Smyth et al., 2006 and Steyn et al., 2013) when CMAQ ozone performed better. Some explanation of these various result would be nice.

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P5608 ln4-6: This is not an accurate statement. The use of the higher minimum eddy diffusivity is not to compensate for “inability to resolve turbulence at smaller scales”. Representing the effects of subgrid turbulence is the purpose of eddy diffusion schemes. This statement implies that they fail in their purpose. I would say that higher minimum eddy diffusivity is sometime used to compensate for specific inadequately modeled effects such as urban heat island as is currently done in CMAQ where a higher minimum eddy diffusivity is used in urban areas.

P5608 ln6-9: I also take issue with this statement concerning the study presented by Pleim and Gilliam (2012). This study used CMAQv5.0.1 where the minimum eddy diffusivity is 0.01 m2/s except in urban areas where it ramps up to 1.0 m2/s. Thus, the values considered in that study over the great majority of grid cells are much lower than are being discussed in this paper. The purpose of that study was to see if the high values in the urban areas could be removed when a simple urban surface parameterization is used. While the results showed marginally worse performance when the high values in the urban areas were removed, there is hope that improved urban schemes will eliminate this need.

P5608 ln9: Change “. . .that in the use of a lower-limit cutoff for the model diffusion coefficients . . .” to “. . .that the use of a greater lower-limit cutoff for the model diffusion coefficients in the air quality model than are used in the meteorology model. . .” Note that all models have some lower limit to eddy diffusivity to avoid numerical errors.

P5621 ln11: terminology here and earlier is confusing. Using “the lower cutoff” implies a lower value but that is opposite of what is meant. Clarify by changing to something like: “a greater value of the minimum eddy diffusivity”

P5622 ln1-3: I disagree with this statement. It should be the goal of all air quality models to use the same PBL model and the same eddy diffusivities as the meteorology model to which it is linked. There is no physical reason to model the turbulent mixing of chemical scalars differently from meteorological scalars. These greater values of the

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minimum eddy diffusivity are simply artifacts which compensate for other errors in the CTM systems. That is not to say that PBL models don't need improvement; they clearly do. But the improvements should be made identically to both the meteorological and CTM systems.

Technical Comments:

P5602 ln6: Change "...in relative..." to "...relative..."

P5607 ln12-25: This paragraph seems to be a repetition of an earlier paragraph. It should be eliminated or reduced.

P5610 ln7: Please clarify "second to 4th largest"

P5612 ln 9: remove "altitude"

P5615 ln7: Change "important" to "importance"

Interactive comment on Geosci. Model Dev. Discuss., 6, 5595, 2013.

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