Assessment of the Effects of Horizontal Grid Resolution on Long-Term Air Quality Trends using Coupled WRF-CMAQ Simulations

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Abstract

The objective of this study is to determine the adequacy of using a relatively coarse horizontal resolution (i.e. 36 km) to simulate long-term trends of pollutant concentrations and radiation variables with the coupled WRF-CMAQ model. WRF-CMAQ simulations over the continental United State are performed over the 2001 to 2010 time period at two different horizontal resolutions of 12 and 36 km. Both simulations used the same emission inventory and model configurations. Model results are compared both in space and time to assess the potential weaknesses and strengths of using coarse resolution in long-term air quality applications. The results show that the 36 km and 12 km simulations are comparable in terms of trends analysis for both pollutant concentrations and radiation variables. The advantage of using the coarser 36 km resolution is a significant reduction of computational cost, time and storage requirement which are key considerations when performing multiple years of simulations for trend analysis. However, if such simulations are to be used for local air quality analysis, finer horizontal resolution may be beneficial since it can provide information on local gradients. In particular, divergences between the two simulations are noticeable in urban, complex terrain and coastal regions.

1 Introduction

Typically, simulations spanning a year or less with regional-scale air quality model simulations are used in air quality planning applications to estimate future air quality but recently many studies are performing longer-term simulations to assess the abilities of these modeling systems in capturing trends in air quality and air quality - meteorology interactions over time periods of decreasing emissions (Hand et al. 2012, Gan et al. 2014, 2015 and Chin et al. 2014). However, one of the challenges in performing such longer-term simulations is computational cost. A variety of strategies have been adopted to meet this challenge. One is to utilize modeling domains of limited geographic extent, but this increases the impact of boundary conditions on the model results (Hogrefe et al., 2011). Another approach is to perform the model simulations at a coarser horizontal resolution (i.e. 36 km) than the 12 km resolution typically used in air quality planning applications. In this study, we investigate this second approach by comparing results from coupled WRF-CMAQ simulations performed over the continental United State (U.S.) for 10 years (2001 - 2010) at horizontal resolutions of 12 and 36 km. We also evaluate the benefits and drawbacks of using coarser horizontal resolution in long-term air quality applications. Both simulations used the same emission inventory and model options.

Section 2 provides a brief overview of the configurations of the coupled model. The results from the comparisons and methodologies are presented in Section 3. Finally, Section 4 discusses the conclusions from our analyses.

2 Model Simulations

Simulations with the two-way coupled WRF-CMAQ model with aerosol feedback are analyzed in this study for 2001 to 2010. The WRF-CMAQ model was configured with WRFv3.4 and CMAQv5.02 (Wong et al. 2012). Two sets of model calculations were performed over a modeling domain covering the Continental U.S. (CONUS). One discretized the domain with grid cells of 36 km by 36 km and another with 12 km by 12 km grid cell resolutions. The vertical domain employed 35 vertical layers of varying thickness (between the surface and 50 hPa). The comprehensive emission data is based on Xing et al. (2013) and the boundary conditions are obtained from a 108 x 108 km WRF-CMAQ hemispheric simulation (Xing et al. 2015). The details of the model configurations are listed in Table 1. In order to make both simulations

comparable with each other, the 36 km simulation was regridded to the 12 km domain using bilinear interpolation for the analysis presented in this study. In this method, each destination point is mapped to a location in the source mesh and the position of the destination point relative to the surrounding source points is then used to calculate the interpolation weights

(http://www.ncl.ucar.edu/Document/Functions/ESMF/ESMF_regrid.shtml). Note that the result of regridding the 12 km fields to the 36 km domain was found to be similar to regridding the 36 km fields to the 12 km domain. Therefore, we present the latter in this manuscript as we are trying to investigate whether using a coarser resolution is sufficient for trend analysis.

3 Methodology and Results

3.1 Temporal Analysis

To determine differences between the two simulations over the course of a year, we computed correlation coefficients and mean differences across space (i.e. non-water grid cell) for daily average all-sky shortwave (SW) radiation at the ground, clear-sky SW radiation at the ground, aerosol optical depth (AOD), and concentrations of total PM_{2.5}, sulfate (SO_4^{2-}), elemental carbon (EC), nitrate (NO_3^-) and ozone (O₃) for 2010. For each day and each variable, one-dimensional data arrays were constructed for both simulations using all non-water grid cells in the 12 km domain and the correlation coefficients and mean differences between these one-dimensional data arrays were then computed. For the calculation of differences, the 12 km results were subtracted from the regridded 36 km results. The resulting time series are shown in Figure 1 (the correlation coefficients are shown in red and use the left y-axis while the differences are shown in blue and use the right y-axis). For all-sky SW radiation, correlations between the two simulations are highest during winter and decrease during summer when convection is stronger. The correlation coefficients decrease to about 0.84 and differences between the two simulations become as high as $\pm 4 \text{ W/m}^2$. The seasonal patterns of correlation coefficients and differences are similar for clear-sky SW radiation but the correlations are higher and the differences are smaller. AOD values for the 12 km simulations tend to be slightly higher than those for the 36 km simulations, especially during spring and summer. The correlation coefficients and differences for total PM_{2.5}, SO_4^{2-} , NO_3^- , EC and O₃ show more intra-seasonal variability than SW radiation

and AOD. While $\text{PM}_{2.5}$, SO_4^{2-} and NO_3^- show both positive and negative differences during all seasons, EC differences are always positive, indicating higher concentrations in the 36 km simulations. In contrast, O_3 values typically are slightly higher in the 12 km simulation. Overall, the time series shown in Figure 1 indicate that systematic differences between the two simulations are relatively small and tend to average out, especially when considering annual averages.

In order to better illustrate systematic seasonal differences between the two sets of simulations, the correlations and differences between maps (i.e. non-water grid cells) of monthly mean values averaged over multiple years (2002, 2003, 2005, 2007, 2008, 2009 and 2010) are computed and presented in Figure 2. Note that we excluded results from 2001, 2004 and 2006 since data from January 2001 and January – April 2004 and 2006 were corrupted and including only partial-year data from those years would have distorted the overall analysis. The results shown in Figure 2 confirm the presence of seasonal variations in correlation coefficients and differences as discussed in the previous paragraph based on 2010 data only.

3.2 Spatial Analysis

In addition to these seasonal cycles, we constructed maps of absolute differences in seasonal average values between the 36 km and 12 km simulations for a typical year. For illustrative purposes, we selected 2010, but the results are similar for other years. Only summer (June, July, and August) and winter (November, December and January) results are shown in Figures 3 and 4 respectively because the differences are more significant in these two seasons. The left column of Figures 3 and 4 shows the differences between the two simulations (i.e. 36 km minus 12 km) while the right column shows seasonal means from the 12 km resolution simulation. The differences of seasonal mean surface concentrations of $\text{PM}_{2.5}$, SO_4^{2-} , NO_3^- , EC and O_3 averaged over all non-water grid cells are relatively small as shown in Table 2. Moreover, the AOD from the 12 km simulation are slightly higher than those from the 36 km simulation but the differences are very small (e.g. summer different: -0.0018 unitless or -4.2 %). Lastly, the comparison of all-sky SW radiation (see Figures 3 (g) and 4 (g)) shows larger differences in coastal areas which may be due to the effects of grid resolution on clouds while the comparison of clear-sky SW radiation (see Figures 3 (i) and 4 (i)) shows smaller impacts of grid resolution that are primarily

in areas of complex terrain. For example, the summer overall mean differences for all-sky and clear-sky SW radiation are less than 1.7 W/m^2 or 0.55% and 0.0094 W/m^2 or 0.003% respectively. The terrain height effect is confirmed in Figure 5 (a) which illustrates the difference of the terrain height between the two resolutions. The contrast is most noticeable in higher terrain areas where terrain difference patterns closely match clear-sky SW radiation differences (see Figure 3 (i) and 4 (i)). In general, our results indicate that the differences tend to be highest in areas of complex terrain, coastlines, and near major emission sources but the approximate percentage of seasonal mean differences between the two simulations over land surface is less than 9% and should not have a strong impact on simulated long-term trends; this is examined in more detail in the following section.

3.3 Trends Analysis

While the results discussed above show that differences do exist between the two simulations for a given year, they do not address the question whether such differences impact inferences on temporal trends simulated by the two different model configurations, the primary metric of interest when performing long-term simulations.

In order to further determine the effects caused by the different resolution, we assess the 10 years summer trends (2001 – 2010) of $\text{PM}_{2.5}$, SO_4^{2-} , AOD and both all-sky and clear-sky SW radiation over the CONUS domain spatially. Note that, since data for several months in winter and spring were corrupted for some years as discussed in Section 3.1, only summer trends (June, July and August) are presented in this discussion. The right panel of Figure 6 shows the trends computed based on the 12 km simulations. These results indicate decreasing trends of SO_4^{2-} , $\text{PM}_{2.5}$ and AOD and an increasing trend of all-sky and clear-sky SW radiation especially in the eastern U.S.. The left panel shows the differences of the trends between the two simulations (i.e. regridded 36 km minus 12 km); the differences are small relative to the absolute 12km trends (see Table 3 for a summary of trends and absolute and percentage trend differences averaged over all non-water grid cells). For example, Figure 6 (j) illustrates that about $0.9 \text{ W/m}^2/\text{year}$ increase of clear-sky SW radiation occurred over the eastern U.S. with the largest increases occurring downwind of the Ohio River Valley, an area that experienced large decreases in SO_2 emissions during this time period (Xing et al., 2013). Figure 6 (i) shows the effect of model

resolution on the trends is much smaller than the trend itself. The same finding holds true for AOD as shown in Figures 6 (e-f), except that the sign of the change is reversed compared to Figures 6 (i-j) since reduced emissions led to reduced aerosol loading and consequently to lower AOD. Moreover, the trend results agree well with the results presented in Gan et al. [2014 and 2015] which utilized only the 36 km simulation. Note that the percent difference of all-sky SW is more significant probably because the cloud simulation is more sensitive to the grid cell and hence leads to higher differences in the all-sky radiation.

To complement the analysis of the trend maps shown in Figure 6, we also computed 10-year trends of spatial average summer mean $\text{PM}_{2.5}$, SO_4^{2-} , NO_3^- , EC, O_3 , AOD and all-sky and clear-sky SW radiation values from both simulations (Table 3). These trends were computed based on a least square fit (LSF) of the summer mean model values averaged over all non-water grid cells depicted in Figure 7. As shown in Figure 7 and Table 3, the results from both resolutions agree well with each other providing confidence that using the 36 km horizontal resolution should be sufficient for long-term air quality applications unless specific assessment of smaller targeted areas such as urban, industrial and highly polluted areas is needed.

4 Conclusion

The results presented in this study show that differences in grid resolution for long-term coupled WRF-CMAQ simulations can have seasonally varying effects on radiation, AOD and $\text{PM}_{2.5}$ concentrations. However, these differences are shown to be relatively small with the largest differences being of an episodic nature. Consequently, longer-term averages tend to be less influenced by differences in model configuration. Moreover, it was shown that changes over time (i.e. long-term trends) in radiation, AOD, and particulate matter concentrations are generally very similar between the 36 km and 12 km model configurations. Considering that the computational burden associated with the 36 km model configuration is roughly seven times lower than that of the 12 km model configuration, the results of this study suggest that using the coarser model resolution is a viable option for long-term simulations and air quality planning applications. Moreover, the storage requirement for the model output is about nine times smaller. In particular, a coarser resolution simulation approach can help to estimate the long-range transport of pollution over larger domains and longer time periods. However, if the focus of the

application is on local sources and features, performing the simulations at finer grid resolution would be preferable (e.g. short-term field campaign studies such as Discover-AQ).

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243 Table 1: List of configurations

Parameter	Configuration
Emission	Xing et al. [2013]
Planetary Boundary Layer	ACM2 (Pleim 2007)
Microphysics	Morrison 2-moment
Gas-phase Chemistry	Carbon Bond 05
Aerosol Chemistry	aero6 (Appel et al., 2013)
Land Surface	Pleim-Xiu
Cumulus	Kain-Fritsch 2
Radiation	RRTMG SW & LW
Land use	NLCD 50
Boundary condition	Xing et al. [2015]

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245 Table 2: Seasonal mean absolute and percentage differences (36 km simulation minus 12 km
 246 simulation) averaged over all non-water grid cells for 2010. Trends for SW radiation are shown
 247 in $W/m^2/year$, for AOD is shown in unitless/year, for ozone is shown in ppbV/year and for
 248 PM_{2.5}, nitrate, sulfate and element carbon are shown in $\mu g/m^3/year$.

Variable	Summer		Winter	
	mean	percent	mean	percent
All-sky SW	1.7022	0.551	0.6840	0.610
Clear-sky SW	-0.0094	-0.003	-0.1545	-0.109
AOD	-0.0018	-4.160	0.0003	0.863
PM _{2.5}	0.1481	2.660	0.1865	1.990
Nitrate	0.0090	8.200	0.0660	3.900
Element Carbon	0.0213	9.420	0.0153	4.396
Sulfate	-0.0286	-2.260	-0.0094	-0.720
Ozone	-0.7025	-1.987	-0.5262	-1.907

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251 Table 3: Least-square fit trends and absolute and percentage trend differences (36 km
 252 simulations minus 12 km simulations) averaged over all non-water grid cells. Summer (June,
 253 July and August) average values for 2001 – 2010 were used in this analysis. Trends for SW
 254 radiation are shown in $W/m^2/year$, for AOD is shown in unitless/year, for ozone is shown in
 255 ppbV/year and for PM_{2.5}, nitrate, sulfate and element carbon are shown in $\mu g/m^3/year$.

Trend	Element					All-sky	Clear-	Ozone
	Carbon	Nitrate	Sulfate	PM _{2.5}	AOD	SW	sky SW	
36 km	-0.003	-0.016	-0.08	-0.16	-0.002	0.273	0.194	-0.003
12 km	-0.0034	-0.0142	-0.0775	-0.1585	-0.0018	0.2182	0.2303	-0.0034
difference	0.0004	-0.0018	-0.0025	-0.0015	-0.0002	0.0548	-0.0363	0.0004
percentage	12.50	11.92	3.17	0.94	10.53	22.31	17.11	12.50

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Figure 1: Time series of correlation coefficients (red, left y-axis) and differences (blue, right y-axis) between the 36 km and 12 km simulation results computed across space from daily average values for 2010. Further details on the computation of these time series are provided in the text.

Figure 2: Time series of correlation coefficients (red, left y-axis) and differences (blue, right y-axis) between the 36 km and 12 km simulation results computed across space from monthly average values. Results were computed individually for 2002, 2003, 2005, 2007, 2008, 2009 and 2010 and then averaged over these seven years for display in this figure to illustrate systematic seasonal variations in correlation coefficients and differences between the simulations. Further details on the computation of these time series are provided in the text.

282 Figure 3: The first column shows the mean differences between the two simulations (36 km
 283 minus 12 km) and the second column shows the absolute values of PM_{2.5}, SO₄²⁻, AOD, all-sky
 284 and clear-sky SW radiation. The results shown here are for the summer (June – August) of 2010.

290 Figure 4: As in Figure 2 but for winter (Nov, Dec and Jan) 2010

Figure 5: The left panel is the difference of the terrain height between the 36 km and 12 km simulations and the right panel is the 12 km terrain height.

321 Figure 6: The first column shows the differences of 2001 – 2010 summer trends in PM_{2.5}, SO₄²⁻,
 322 AOD, all-sky and clear-sky SW radiation between the two simulations (36 km trend minus 12
 323 km trend) and the second column shows the corresponding trends from the 12 km simulation.

Figure 7: (a) Summer (June, July and August) mean values spatially averaged over all non-water grid cells for the 12 km and 36 km simulation.s (a) all-sky and clear-sky SW radiation (both on the left axis) and AOD (right axis). (b) EC, NO_3^- , SO_4^{2-} and $\text{PM}_{2.5}$ (left axis) and O_3 (right axis).