Improvements to the WRF-CMAQ Modeling System for Fine-Scale Air Quality Simulations: Application to the DISCOVER-AQ Baltimore/Washington D.C. Campaign

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Background

Despite significant reductions in atmospheric pollutants such as ozone (O_3) and fine particulate matter ($PM_{2.5}$) over the past several decades, air pollution continues to pose a threat to the health of humans and sensitive ecosystems. A number of areas across the U.S. remain in violation of the National Ambient Air Quality Standards (NAAQS; http://www.epa.gov/airquality/greenbook). Numerical air quality modeling systems designed to simulate the emissions, transport and fate of atmospheric pollutants are a critical part of the regulatory process in designing abatement strategies to reduce these pollutants. Air quality models are also used to forecast "next day" air quality conditions so as to allow citizens to modify their activities accordingly to avoid potential health issues (e.g. asthma attacks).

Eulerian air quality models, such as the Community Multiscale Air Quality (CMAQ; Foley et al. 2010) model, discretize large simulation domains into smaller sized grid cells in order to better represent spatial heterogeneities, with smaller-sized grid cells in theory providing a truer representation of fine-scale processes and near-field impacts. While utilizing larger-sized grid cells has the advantage of minimizing computation resources, it does have several disadvantages. Since Eulerian air quality models instantly dilute point emissions across the entire volume of the grid cell, decisions on grid resolution should be made with consideration of the spatial scale of the air quality problem, meteorology, and emissions being modeled while also recognizing the increased computation resources required as grid cell size is decreased. The smaller the dimensions of the grid cells used, the more representative the model may be of the actual point source emissions. Additionally, meteorological fields (e.g. wind and temperature) are also likely to be better represented with smaller grid cells, particularly in areas with diverse and complex geography (e.g. coastal and mountainous regions).

The goals of this work are two-fold. First, to demonstrate the application and skill of the coupled WRF-CMAQ modeling system (Wong et al., 2012) at fine-scales (i.e. 4 and 1 km). Second, to evaluate the model results of the various simulations against a high-quality meteorological and air quality observation dataset. To meet these goals, model simulations are performed using 12-km, 4-km and 1-km horizontal grid spacing (Figure 1) over the continental U.S. (12-km domain), a portion of the eastern U.S. (4-km domain) and the Baltimore/Washington D.C. region (1-km domain). The results from the simulations are then compared to measurements from the Baltimore/Washington D.C. DISCOVER-AQ campaign in 2011 (http://www.nasa.gov/mission_pages/discover-aq/index.html). Discussed here are several innovative modeling techniques and new data sets that were required to produce fine-scale WRF-CMAQ model simulations that performed at least as well as the coarser 12-km model simulation.

Iterative WRF analysis for fine-scale applications

For retrospective simulations, such as performed here, the Weather Research and Forecasting meteorological model (WRF; Skamarock et al., 2008) is typically run using four-dimensional data assimilation (FDDA), which requires gridded analyses of wind, temperature and moisture to nudge the atmosphere above the planetary boundary layer (PBL). Also used are 2-m temperature and moisture analyses that are fused with surface observations to indirectly nudge soil moisture and temperature so that the ground-level WRF fields more closely track the observations.

For this application, the readily available North American Model analysis product at 12-km horizontal grid spacing (NAM-12) was used for the initial WRF model applications for all three domains (12-km, 4-km and 1-km). The 2-m analysis data are only used to directly adjust the soil temperature and moisture fields and not the atmosphere within the PBL. While the model performance for the 12-km simulation was consistent with results from comparable 12-km WRF simulations, the model performance for the initial 4-km and 1-km simulations was poor compared to that of the 12-km simulation, as the coarse input data from the NAM-12 reanalysis product was inadequate (and perhaps even harmful) for the fine-scale WRF simulations.

In order to improve the near-surface analysis fields used to adjust soil temperature and moisture, an iterative process for running WRF at fine-scales was developed. Simply described, an initial 1-km or 4-km WRF simulation is performed using the coarse input data available from the NAM-12 as the analysis field. Once that run is complete, a second WRF simulation is performed using the output from the initial WRF simulation in place of the NAM-12 data used in the initial WRF simulation. These first guess fields are then fused with observations to correct for model bias. While the NAM-12 analysis is quite coarse with few discernable topographic features (Figure 2), the 1-km and 4-km iterative analysis fields have a much more realistic representation of the gradients in temperature caused by the Chesapeake Bay and other topographic features (Figure 2). The 2-m temperature error is also greatly reduced in the iterative WRF simulations (Figure 3).

Improved representation of urban environments

Urban landscapes present other challenges that standard WRF configurations do not resolve well. The numerous tall buildings disturb wind flow more than natural landscapes, and radiation is trapped through multiple reflections between building walls. Additionally, urban areas have relatively high heat capacity due to abundant cement and asphalt that can make up the majority of the city landscape. Such surfaces require more radiative energy to warm early in the day as the sun rises, reach peak temperature later in the day and cool slower in the evening than more natural surfaces found outside of cities (e.g. grasslands, forests, and agricultural fields). The net impact on the meteorology and air quality is slower buildup of O_3 in the morning due to slower entrainment from layers aloft and greater titration of O_3 by NO_x which is less diluted in the more slowly deepening mixed layer. In the late afternoon and early evening, cooling and stabilizing occurs more slowly in the urban boundary layer thereby increasing dilution of surface emitted pollutants such as NO_x resulting in less titration and greater concentrations of O_3.

In order to address the deficiencies of standard WRF-CMAQ simulations in properly representing urban areas a simple approach was applied which leverages very accurate and highly resolved impervious surface and canopy fraction data that are available from the National Land Cover Database (NLCD). In addition, the NLCD includes four urban classes for which surface characteristics can be differentially assigned. For example, in the three urban categories that represent high, medium, and low density developed areas of cities from the urban core to the suburbs, surface roughness is increased to better account for the effects of structures and the albedo is decreased to account for the effects of radiation trapping within urban street canyons. Next, the impervious surface data are gridded to the WRF domain and the fraction of impervious surface in each model grid cell is used to adjust the volumetric heat capacity of the surface. Previously, the heat capacity was only based on fraction of vegetation versus natural ground surface. Now the percent impervious surface is considered and the remainder is split between vegetation and bare ground to give a weighted value for the grid cell's surface heat capacity. For the impervious fraction, the heat capacity was based on civil engineering estimates for asphalt and concrete with thickness of about 15 cm. Furthermore, since the urban land use categories do not give information about vegetation coverage, which is critically important to realistic partitioning of sensible and latent surface heat flux, the forest canopy fractional coverage is used along with the imperious fraction to constrain the forest and other vegetation fractions and better estimate the grid cell aggregate leaf area index (LAI). In future work, anthropogenic heating from traffic, residential heating and cooling, and commercial and industrial sources will be added. These effects will be particularly important during the winter in colder climates.

Figure 3 shows the change in 2-m temperature error (all hours) between the base WRF simulation and the WRF simulation with the changes to account for the effects of the urban environments. As expected, the largest reductions in error occur in the most highly urbanized areas, specifically in and around the Washington D.C. and Baltimore MD regions. The model typically cools these urban areas too quickly in the evening and overnight, but accounting for the increased heat capacity of the urban environments retains the heat longer resulting in a reduction of the overnight cool bias that is often present in the summer.

High-resolution sea-surface temperature fields

The final change made to improve the fine-scale WRF simulation was an update to the sea-surface temperature (SST) data used. For the 12-km WRF simulations, SST data were obtained from the NAM-12. However, it was evident in the 1-km WRF simulations that the relatively coarse NAM-12 SST data were not representing the temperature gradients across the Chesapeake Bay very well, often resulting in areas of erroneously cold surface temperatures (Figure 4). To improve the simulated temperature in and around the bay, and consequently an improved representation of the land-bay breeze, a more detailed SST data set was needed. The Group for High-Resolution SST (GHR-SST; https://www.ghrsst.org/) product from the Advanced Very-High Resolution Radiometer (AVHRR) satellite provides twice daily composite SST measurements at 1-km grid spacing. When these data were used in place of the NAM-12 SST data, the representation of Chesapeake Bay and its many smaller inlets and tributaries was improved significantly (Figure 4). A comparison of the 2-m temperature error between the WRF simulations using the NAM-12 SST data and the GHR-SST data show a significant reduction in the error in the WRF simulation using GHR-SST.

Application of WRF-CMAQ at 12-km, 4-km and 1-km resolutions

Table 1 presents summary statistics for July 2011 for the three grid resolutions for hourly O_3 and $PM_{2.5}$ for all sites in the 1-km domain. For O_3, the 1-km performed better than the 12-km and 4-km simulations in terms of correlation (r) and root mean square error (RMSE), normalized mean error

(NME) and mean error (ME), but worse for normalized mean bias (NMB) and mean bias (MB). For $PM_{2.5}$, the opposite is the case, with the 1-km performing worse than the 12-km and 4-km simulations in terms of r and error, but having the best performance of the three simulation in terms of bias. It's not immediately apparent why the 1-km simulation has higher error for $PM_{2.5}$ than the 12-km and 4-km simulations, and additional analysis is needed to determine what changes may need to be made (e.g. emissions) to improve the 1-km performance for $PM_{2.5}$.

Figure 5 shows a comparison of O_3 and 10-m wind vectors for July 2 at 5PM local time for all three domains. The representation of the bay breeze and sea breeze appears more realistic and better defined in the 4-km and 1-km simulations than the 12-km, in which it is difficult to identify the extent of the bay and sea breezes. The 4-km and 1-km simulations also tend to compare better with the observed O_3 mixing ratios (shown in the circles), particularly around the Washington D.C. and Baltimore, MD regions. Additional analysis is needed to determine quantitatively how the representation of the bay and sea breezes compare between the different model resolutions for the entire month. Overall however, the model performance for the finer-scale simulations is somewhat better for O_3 and somewhat worse for $PM_{2.5}$ compared to the regional scale simulation, demonstrating the successful application of the WRF-CMAQ modeling system at fine-scales. More analysis is needed to determine where and when the model performance of the finer-scale simulations improves upon the performance of the regional scale simulation.

Summary

The WRF-CMAQ modeling system has been applied at 12-km, 4-km and 1-km horizontal grid spacing to the 2011 DISCOVER-AQ campaign for the Baltimore MD, Washington D.C. region. To improve the finer-scale WRF simulations several advances in the input processing and execution of the WRF model were made. First, an iterative processing technique was applied in which 1-km resolution WRF model output is recycled to serve as background for a much more accurate 1-km re-analysis that is then used for soil moisture and temperature data assimilation. The second improvement applied was the incorporation of high-resolution impervious surface, tree canopy, and land-use data to improve the representation of the urban environment (e.g. buildings and pavement) to better represent the urban heat-island effect. Finally, a high-resolution 1-km SST dataset was acquired to replace the coarse 12-km SST dataset that is typically used for regional scale WRF applications. Together, these improvements to the WRF-CMAQ modeling system resulted in a dramatically improved 1-km simulation of meteorology compared to the initial 1-km simulation without these improvements.

Aggregate model performance metrics for hourly O_3 and $PM_{2.5}$ were generally similar between the three grid resolutions averaged across the entire month, with the 1-km simulation having slightly less error (but slightly more bias) for O_3 than the 12-km and 4-km simulations, while for $PM_{2.5}$ the 1-km had slightly less bias but greater error than the 12-km and 4-km simulations. Future work will include detailed comparisons of the model outputs with some high space and time resolved measurements made during the DISCOVER-AQ campaign, such as ship measurements made over the Chesapeake Bay and extensive aircraft measurements taken over the Baltimore region. Additional comparisons of the model results to the DISCOVER-AQ measurements will focus on assessing the accuracy of vertical mixing and horizontal transport (aloft) in the model.

Disclaimer

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Table 1. Summary statistics for the 12-km, 4-km and 1-km WRF-CMAQ model simulations. All statistics are based on only the AQS sites that fall within the 1-km domain (12-km and 4-km domains are windowed to the 1-km).

Domain	r	RMSE	NMB	MB	NME	ME
			O_3			
1km	0.76	14.6	-1.4	-0.61	26.6	11.1
4km	0.74	15.3	-1.7	-0.7	27.7	11.6
12km	0.74	15.7	0.1	0.03	28.2	11.8
			$PM_{2.5}$			
1km	0.22	18.6	-8.8	-1.46	58.5	9.73
4km	0.38	11.1	-16.6	-2.76	47.7	7.94
12km	0.41	10.6	-25.9	-4.36	48.2	8.1

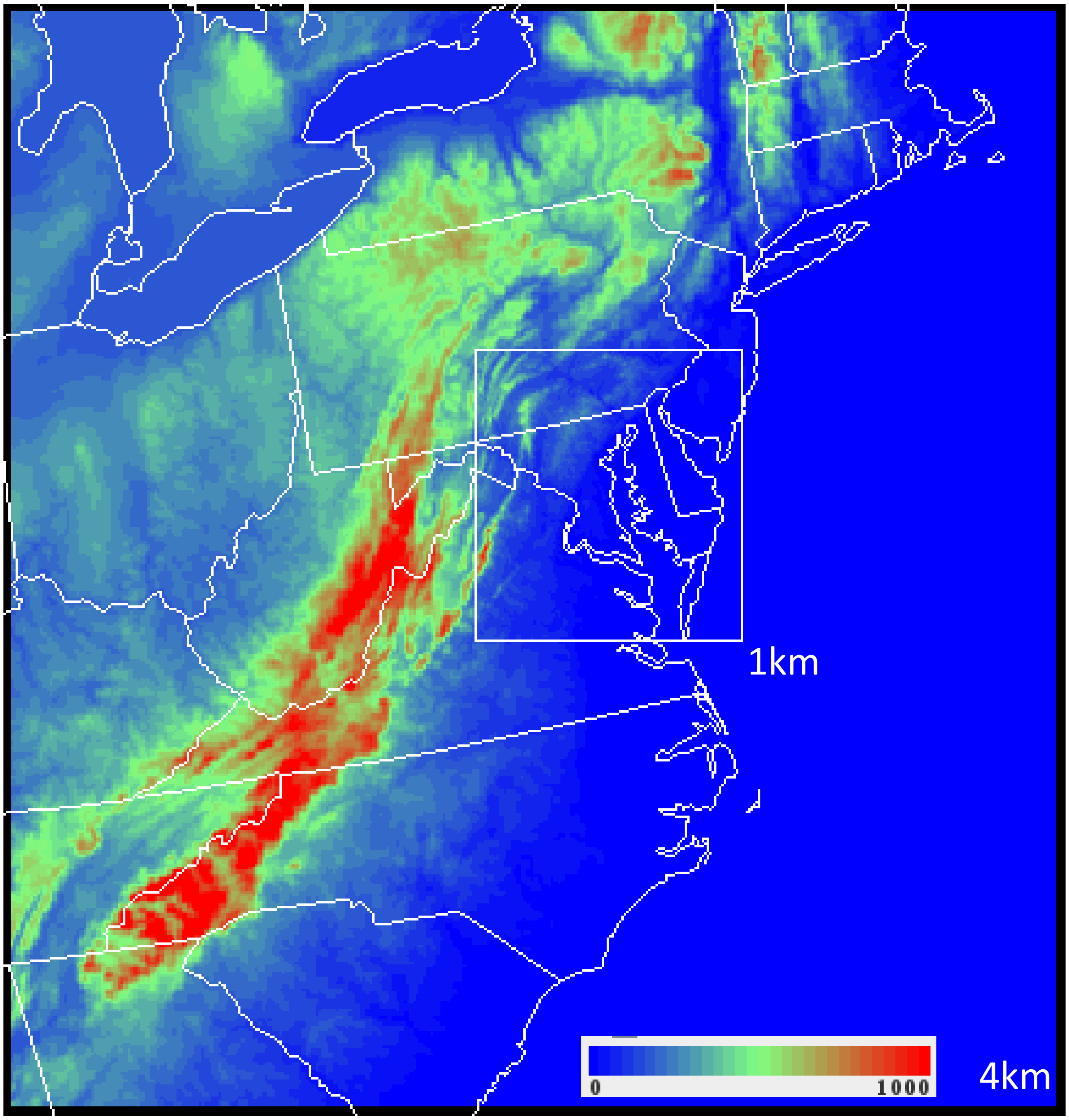

Figure 1. Depiction of the 4-km and 1-km WRF-CMAQ domains (terrain height shown in meters). The 12-km domain (not shown) covers the entire continental U.S., including southern Canada and northern Mexico.

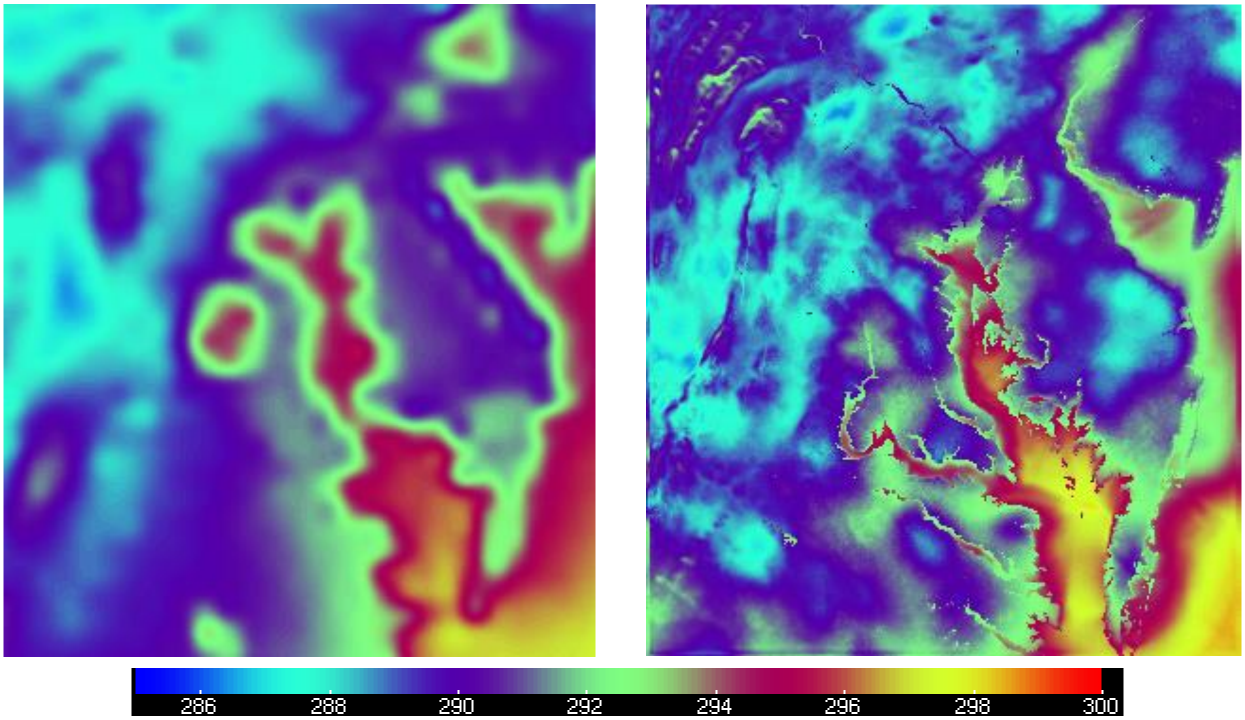

Figure 2. Left, 2-m temperature (K) analysis field for soil nudging using NAM 12-km background. Right, 2-m temperature (K) analysis field for soil nudging using iterative 1-km WRF output as background.

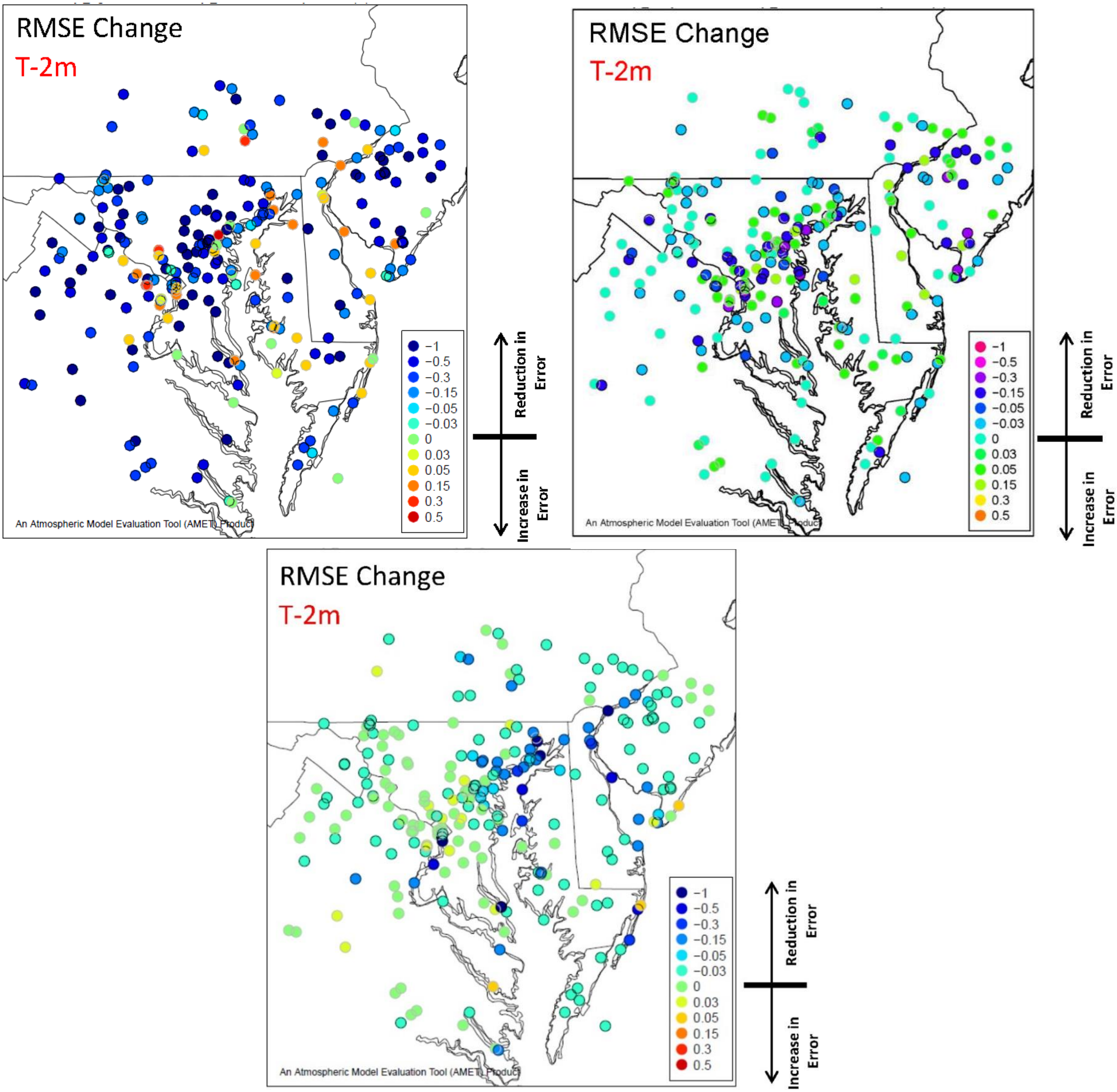

Figure 3. Top left: change in 2-m temperature (K) error for the 1-km WRF simulation due to the iterative WRF processing. Top right: change in 2-m temperature (K) error for the 1-km WRF simulation due to inclusion of impervious surface and urban canopy parameterizations. Bottom: change in 2-m temperature (K) for the 1-km WRF simulation for July due to inclusion of the GHRSST data.

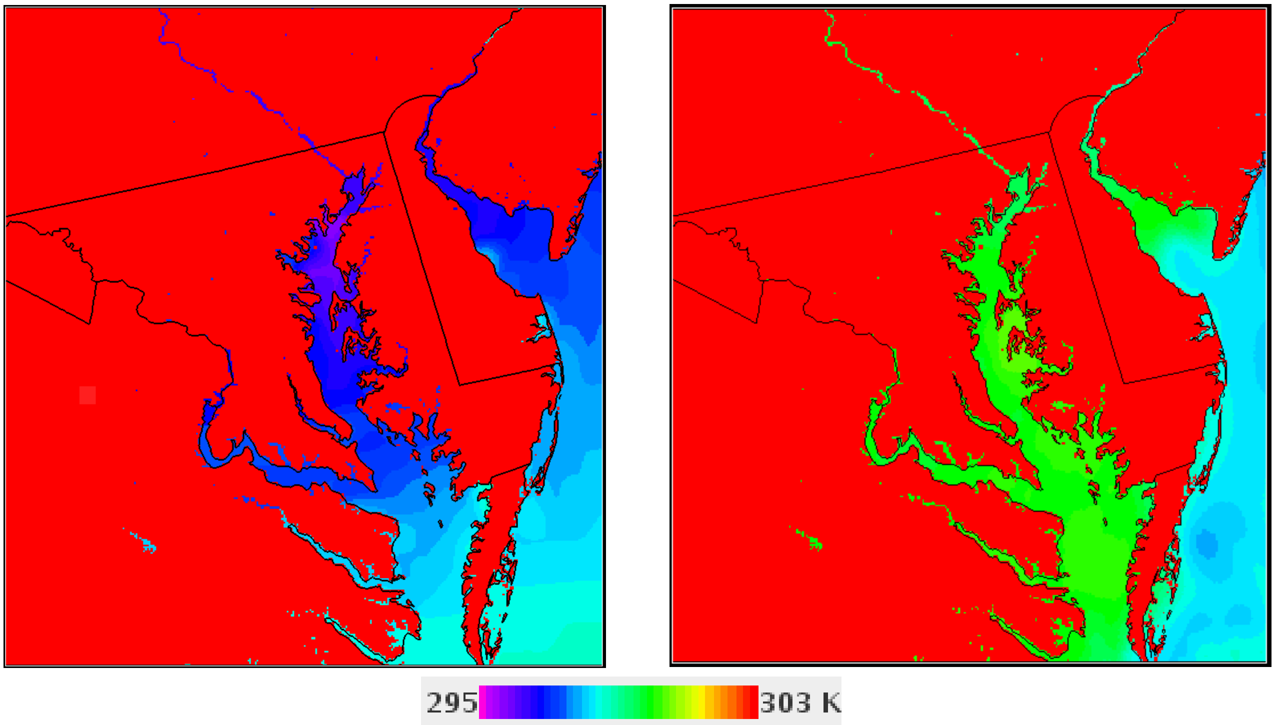

Figure 4. Left, skin temperature (K) field using the NAM 12-km data. Right, skin temperature (K) field using the GHR-SST 1-km data.

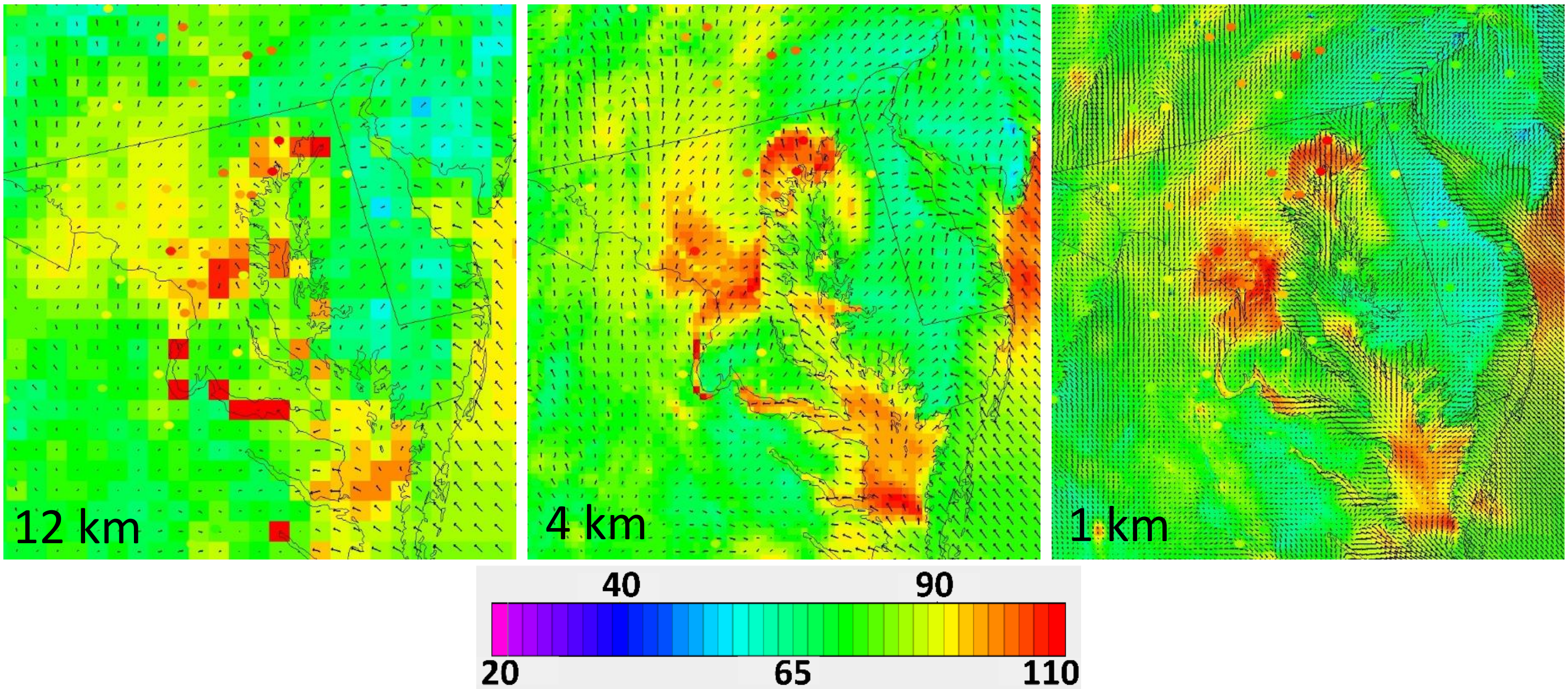

Figure 5. Ozone mixing ratio (shading; 20-110 ppb) and 10-m wind vectors for 2 July 2011 at 5PM local time using 12-km (left), 4-km (center) and 1-km (right) horizontal grid spacing. The 12-km and 4-km results have been windowed to the 1-km domain.