

# Simulating smoke transport from wildland fires with a regional-scale air quality model: Sensitivity to uncertain wind fields

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[1] Uncertainties associated with meteorological inputs which are propagated through atmospheric chemical transport models may constrain their ability to replicate the effects of wildland fires on air quality. Here, we investigate the sensitivity of predicted fine particulate matter (PM<sub>2.5</sub>) levels to uncertain wind fields by simulating the air quality impacts of two fires on an urban area with the Community Multiscale Air Quality modeling system (CMAQ). Brute-force sensitivity analyses show that modeled concentrations at receptors downwind from the fires are highly sensitive to variations in wind speed and direction. Additionally, uncertainty in wind fields produced with the Weather Research and Forecasting model was assessed by evaluating meteorological predictions against surface and upper air observations. Significant differences between predicted and observed wind fields were identified. Simulated PM<sub>2.5</sub> concentrations at urban sites displayed large sensitivities to wind perturbations within the error range of meteorological inputs. The analyses demonstrate that normalized errors in CMAQ predictions attempting to model the regional impacts of fires on PM<sub>2.5</sub> levels could be as high as 100% due to inaccuracies in wind data. Meteorological drivers may largely account for the considerable discrepancies between monitoring site observations and predicted concentrations. The results of this study demonstrate that limitations in fire-related air quality simulations cannot be overcome by solely improving emission rates.

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## 1. Introduction

[2] Wildland fires may greatly impact air quality and pose a significant threat to public health [Delfino *et al.*, 2009]. The adverse effects of smoke from wildfires and prescribed burns on air pollution levels and visibility have been investigated in numerous studies [Fox and Riebau, 2009; Johnston *et al.*, 2012; Kochi *et al.*, 2010]. Air quality models can serve as tools to quantify exposure to fire-related pollution and provide important information to fire and land managers. However, the limitations inherent to numerical models when used to replicate the air quality impacts of fires must be identified and well understood to adequately interpret results and further improve the models' predictive skills.

[3] Multiscale atmospheric chemical transport models provide an appealing framework to simulate the effects of wildland fires on air quality: complex chemical and physical processes are represented; local and regional scales can be jointly

treated; and detailed emissions and meteorological fields can be used to drive air quality modeling. Multiple attempts to replicate the impacts of fires on air quality with Eulerian models have been reported [Goodrick *et al.*, 2012]. Commonly, model performance in these simulations, assessed by comparing forecasted and observed pollutant concentrations, has been unsatisfactory and a need to improve predictions has been recognized.

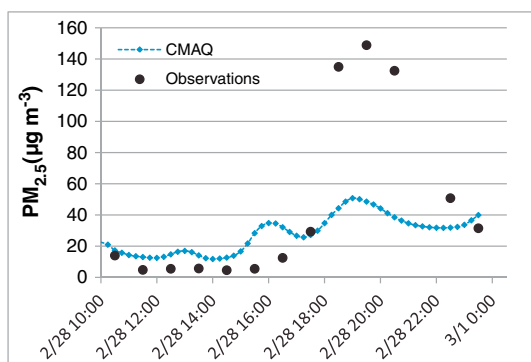
[4] Air quality models require two fundamental inputs: meteorological fields and emission rates. The importance of meteorological input fields in air quality simulations has long been acknowledged [Seaman, 2000]. However, prior studies seeking to simulate the impacts of wildland fires with Eulerian air quality models have generally focused on better characterizing fire-related emissions as a strategy to strengthen model performance [Konovalov *et al.*, 2011; Tian *et al.*, 2009; Yang *et al.*, 2011]. In contrast, little attention has been given to the implications uncertain meteorological inputs may have on model predictions. Still, weather conditions determine the principal physical driving forces in the atmosphere, making gridded representations of meteorology the foundation of all three-dimensional air quality simulations. While enhanced fire emissions estimates can improve the accuracy of air quality simulations, errors associated with weather data continue to affect model results. Therefore, determining the degree to which uncertainties in meteorological inputs might hinder fire-related simulations is an important step towards successfully modeling the impacts of wildland fires on pollutant levels with atmospheric chemical transport models.

Additional supporting information may be found in the online version of this article.

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**Figure 1.** Observed 1 h average and CMAQ-predicted 15 min PM<sub>2.5</sub> concentrations at the Confederate Ave. monitoring site on 28 February 2007 (LT).

[5] Sensitivity analyses are an important diagnostic tool to evaluate the influence individual inputs may have on specific model outputs. Here, we use a regional-scale chemical transport model to simulate smoke transport from wildland fires in an urban smoke episode which severely deteriorated air quality throughout the Atlanta metropolitan area in 2007. The simulation results show a significant response in predicted PM<sub>2.5</sub> concentrations to small variations in the spatial allocation of fire emissions, suggesting a potentially strong influence from wind inputs. In fact, errors in model-predicted PM<sub>2.5</sub> concentrations could be dominated by the uncertainty in wind fields rather than emission estimates [Yang *et al.*, 2011]. In this paper, the Atlanta 2007 simulation is used as a base case episode to investigate the sensitivities of model predictions to the meteorological fields used to drive air quality simulations.

[6] A series of sensitivity analyses were applied to explore the responsiveness of PM<sub>2.5</sub> concentrations predicted by the air quality model to uncertainties in three-dimensional wind fields. We focus on primary fine carbonaceous particle emissions from fires, the main component of fire-related smoke, and wind, the meteorological variable most clearly associated with fire-attributable impacts on PM<sub>2.5</sub> concentrations. The results of this work indicate the extent to which simulations may be constrained by inaccuracies in meteorological data produced by numerical weather prediction models. Additionally, the analysis described in this study investigates whether the errors in predicted concentrations can be abated by exclusively focusing on better estimation of fire-related emissions. The air quality modeling framework used is

described in section 2. Section 3 presents the methodology applied to carry out the sensitivity analyses and evaluate the wind field inputs. The results of the sensitivity analyses and wind field uncertainty assessment are included in section 4. Finally, our conclusions are presented in section 5.

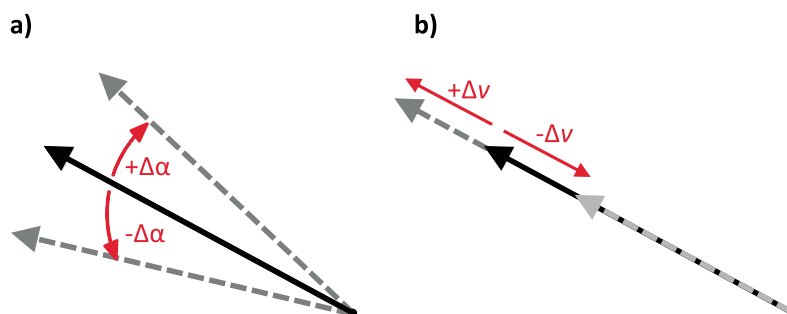
## 2. Numerical Modeling Framework

### 2.1. Meteorology

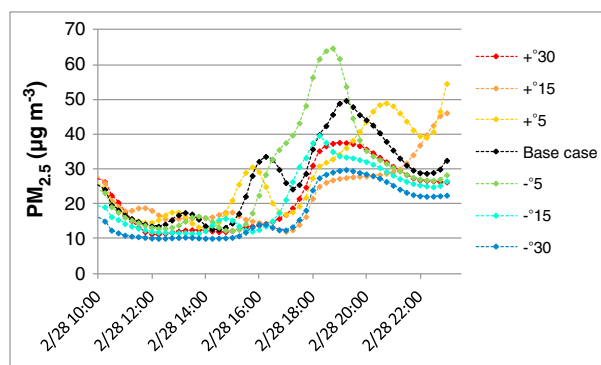
[7] Meteorological data are used to capture atmospheric conditions throughout modeling domains and play a vital role in determining pollutant concentrations predicted by air quality models. Although air quality simulations, particularly those performed with plume or puff models, can rely on observed or simplified weather data, comprehensive Eulerian models require detailed three-dimensional meteorological fields. Meteorological fields used by atmospheric chemical transport models are typically prepared with meso-scale numerical weather prediction systems such as the fifth-generation Pennsylvania State University/National Center for Atmospheric Research Mesoscale Model (MM5; [Grell *et al.*, 1994]) and the Weather Research and Forecasting model (WRF; [Skamarock *et al.*, 2008]). For retrospective air quality simulations, reanalysis fields and data assimilation of observed meteorology can be applied.

[8] Most reported simulations attempting to replicate the impacts of wildland fires on air quality with Eulerian models have relied on meteorological fields produced with MM5 [e.g., J Chen *et al.*, 2008; Junquera *et al.*, 2005; Strand *et al.*, 2012]. The choice is consistent with the initial application of current models, originally designed to use MM5-derived meteorological inputs. More recently, air quality modeling has incorporated meteorological fields generated with WRF [Appel *et al.*, 2010]. Studies comparing MM5 and WRF performance and assessing the sensitivity of air quality predictions to weather model selection indicate that, although differences exist in model results, meteorological and air quality fields based on either are of comparable qualities [Appel *et al.*, 2010; Gilliam and Pleim, 2010].

[9] For this study, meteorological fields produced with WRF (version 2.1.2) were used to drive all air quality modeling. Meteorology was simulated on three nested domains with 36, 12, and 4 km horizontal grid spacing and 34 vertical layers extending up to 50 hPa. The simulations used the Yonsei University planetary boundary layer (PBL) scheme [Hong *et al.*, 2006], Noah land surface model [Ek *et al.*, 2003], Dudhia shortwave radiation scheme [Dudhia, 1989],



**Figure 2.** Representation of perturbations applied to (a) wind direction and (b) wind speed in brute-force sensitivity analyses.



**Figure 3.** CMAQ-predicted PM<sub>2.5</sub> concentrations at the Jefferson St. monitoring site using wind direction perturbations on 28 February 2007 (LT). Base case simulation results are also included.

Rapid Radiative Transfer Model longwave radiation scheme [Mlawer *et al.*, 1997], Kain-Fritsch cumulus parameterization scheme [Kain, 2004], and the Lin *et al.* microphysics scheme [S H Chen and Sun, 2002; Lin *et al.*, 1983; Rutledge and Hobbs, 1984]. The options selected correspond to the configuration of an operational air quality forecasting system in Atlanta which has been used by forecasters in the state of Georgia (USA) since 2006 [Hu *et al.*, 2010]. Simulations were initialized, constrained at the boundaries, and nudged at 6 h intervals using reanalysis fields from the North American Mesoscale model (nomads.ncdc.noaa.gov).

## 2.2. Air Quality

[10] The Community Multiscale Air Quality Modeling system (CMAQ version 4.5, <http://www.cmaq-model.org/>) was used to numerically simulate the transport and transformation of pollutant emissions. Emission inputs from nonfire sources were processed with the Sparse Matrix Operator Kernel Emission processor (SMOKE version 2.1, <http://www.smoke-model.org/index.cfm>). Emission rates for wildland fires featured in the simulated urban smoke episode were prepared through the Fire Emissions Production Simulator (FEPS version 1.1.0, <http://www.fs.fed.us/pnw/fera/feps/>). FEPS provides hourly emissions and heat release rates for prescribed burns or wildfires. Plume rise estimates from the Daysmoke model [Achtemeier *et al.*, 2011] were used to vertically distribute fire emissions. Analogous to the WRF simulations, CMAQ air quality modeling was performed using three levels of nested grids at 36, 12, and 4 km horizontal grid resolutions. Sensitivity analyses relied on simulations carried out with 4 km resolution.

## 3. Methodology

### 3.1. Base Case Simulation

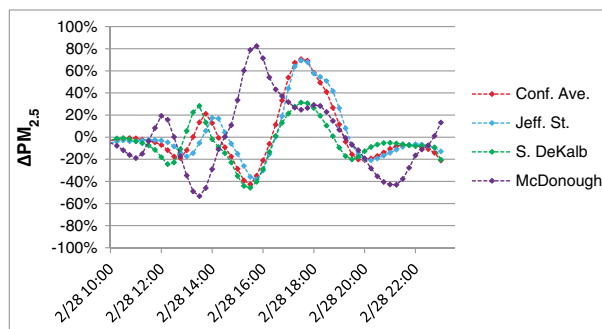
[11] The sensitivity analyses performed were based on a CMAQ simulation of a fire-related smoke episode which occurred on 28 February 2007. The base case air quality simulation intends to replicate the impact of two prescribed burns on PM<sub>2.5</sub> concentrations throughout the Atlanta metropolitan area. The fires occurred at the Oconee National Forest and Piedmont National Wildlife Refuge (henceforth referred to as Oconee and Piedmont), approximately 80 km southeast of Atlanta (see supporting information, Figure S1). Transport

of fire-related emissions by southeasterly winds throughout the day is believed to have led to large increases in pollutant concentrations recorded at urban monitoring sites.

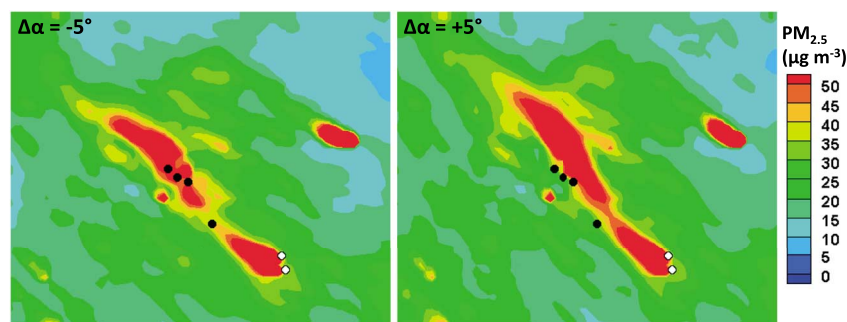
[12] Measured PM<sub>2.5</sub> concentrations from the Georgia Department of Natural Resources' Ambient Monitoring Program and the Southeastern Aerosol Research and Characterization (SEARCH) Network were used to assess model performance. Air quality records from three Atlanta sites (Confederate Ave., Jefferson St., and South DeKalb) and one additional site (McDonough), located approximately midway between Atlanta and the Oconee and Piedmont fires, were considered. Figure 1 shows observed and CMAQ-predicted PM<sub>2.5</sub> concentrations at the Confederate Ave. station. Simulated PM<sub>2.5</sub> concentrations were much lower than observed peaks at monitoring sites. It should be noted that a simulation without the fires predicts about 20 µg m<sup>-3</sup> of PM<sub>2.5</sub> at the Atlanta sites considered, leaving only about 30 µg m<sup>-3</sup> associated with the burns. Consistent with previously reported efforts to replicate the air pollution impacts of wildland fires with Eulerian chemical transport models, the base case CMAQ simulation significantly underpredicts the impacts of prescribed burns on PM<sub>2.5</sub> concentrations observed at urban monitoring stations [Liu *et al.*, 2009; Strand *et al.*, 2012; Yang *et al.*, 2011]. For predicted PM<sub>2.5</sub> levels to match maximum observed concentrations throughout Atlanta, fire emissions would have to be increased by more than 400%. Uncertainties in fire-related emission rates may play a significant role in the underestimation of PM<sub>2.5</sub> concentrations. However, an increment of this magnitude does not seem realistic. In addition, significant sensitivities of CMAQ predictions to the spatiotemporal allocation of fire-related emissions on gridded domains were observed. These are suggestive of potentially important sensitivities to meteorological inputs and in particular to wind fields.

### 3.2. Brute-Force Sensitivity Analyses

[13] A brute-force method was applied to carry out sensitivity analyses. The method relies on successively simulating the same system of interest while varying a specific model input and holding others constant to observe the response of model outputs [Hwang *et al.*, 1997]. In air quality modeling, brute-force sensitivity analyses have been frequently used to quantify the responsiveness of simulated concentrations to changes in emissions. The response of modeled PM<sub>2.5</sub>



**Figure 4.** Change in CMAQ-predicted PM<sub>2.5</sub> concentrations on 28 February 2007 (LT) relative to base case simulation at the Confederate Ave., Jefferson St., South DeKalb, and McDonough monitoring sites after applying a  $-5^\circ$  perturbation to wind direction.



**Figure 5.** CMAQ-predicted PM<sub>2.5</sub> concentrations ( $\mu\text{g m}^{-3}$ ) over northern Georgia at 1900 LT on 28 February 2007 using  $-5^\circ$  and  $+5^\circ$  perturbations to wind direction. Black shaded circles indicate monitoring station locations. The Oconee and Piedmont fire sites are denoted by white shaded markers.

concentrations to changes in primary emissions should be nearly linear [Koo *et al.*, 2009]. Here, the brute-force method is used to assess the sensitivity of simulated PM<sub>2.5</sub> concentrations to perturbations in wind inputs, namely wind speed and direction. In this case, the response of concentrations to changes in winds is not expected to be linear as there are complex nonlinear relationships between the winds and concentrations at downwind receptors. Nevertheless, sensitivity analyses were performed to observe the degree to which simulations are affected by variations, or uncertainty, in wind fields.

[14] A series of simulations under perturbed wind fields were carried out to examine the responsiveness of CMAQ-predicted PM<sub>2.5</sub> concentrations at specific downwind receptors. Wind fields were modified within the Meteorology-Chemistry Interface Processor (MCIP, version 3.4.1, [Otte and Pleim, 2010]) used to convert WRF output fields into CMAQ-compatible inputs. The magnitude and direction of wind vectors read in from WRF-generated fields were perturbed to varying extents to produce modified CMAQ inputs, as illustrated in Figure 2. In this manner, perturbations are reflected in all wind-associated variables included in the meteorological input data used to drive the air quality model. It is also important to note that in CMAQ 4.5, mass conservation is ensured by adjusting vertical winds [Hu *et al.*, 2006]. Perturbations to wind direction and wind speed are accompanied by changes to the vertical winds as mass conservation is obeyed within the model. In general, we find that perturbing horizontal wind speeds leads to proportional changes in the vertical speeds, while the effect of altering wind direction on the vertical wind field is nonlinear and spatially complex.

### 3.3. Meteorological Uncertainty

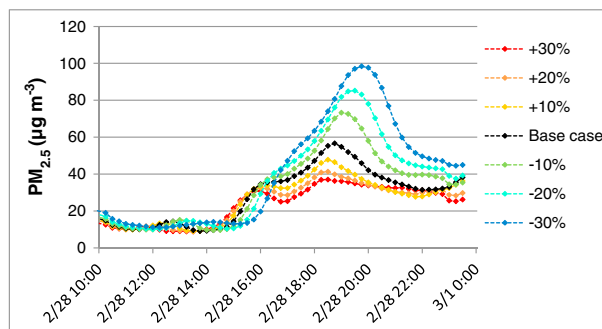
[15] Meteorological model performance was evaluated to assess the level of uncertainty in weather fields used to drive air quality simulations. Hourly surface observations from the Research Data Archive of the National Center for Atmospheric Research (<http://rda.ucar.edu/datasets/ds472.0/>) were used to compute model performance metrics by comparing surface-layer observations and predictions. Bias and error in WRF-derived ground-level predictions were estimated for wind direction, wind speed, temperature, and humidity. Additionally, upper air model predictions were evaluated against atmospheric soundings launched from Peachtree City, GA, approximately 45 km southwest of Atlanta and 80 km northwest from the Oconee and Piedmont fires. Sounding observations were available every 12 h at 0000 and 1200 UT.

## 4. Results

### 4.1. Sensitivity Analyses

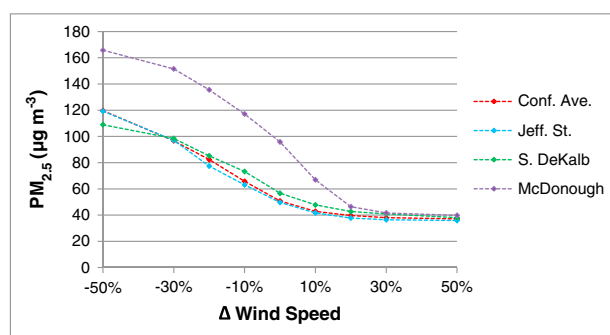
#### 4.1.1. Wind Direction

[16] To examine the sensitivity of CMAQ-predicted PM<sub>2.5</sub> concentrations to wind direction, the Atlanta 2007 smoke episode was modeled under a series of perturbed wind fields. Modified fields were produced by uniformly perturbing wind direction by  $\pm 5^\circ$ ,  $\pm 15^\circ$ , and  $\pm 30^\circ$  across the entire domain. The changes were applied at each grid point by rotating all wind vectors from WRF by the same angle during MCIP processing, as described in section 3.2. A sample of base case and perturbed wind fields is included in Figure S2 in the supporting information. At selected downwind monitoring sites, predicted PM<sub>2.5</sub> concentrations for each perturbed wind field and the base case were compared to observe the responsiveness to variations in wind direction. Figure 3 shows PM<sub>2.5</sub> concentrations simulated by CMAQ at the Jefferson St. monitoring site with both perturbed and unperturbed fields. The sensitivity of predicted PM<sub>2.5</sub> concentrations to wind direction is extremely high at Jefferson St., as well as at all other sites considered. The results indicate that small variations in wind direction can lead to large changes in predicted pollutant concentrations at specific receptors downwind. At Jefferson St., for instance, a  $-5^\circ$  rotation to wind vectors increases the maximum predicted PM<sub>2.5</sub> concentration by more than  $13 \mu\text{g m}^{-3}$ , a 26% increase. At different urban locations, sensitivities to wind direction are likewise large and nonlinear. Peak PM<sub>2.5</sub> concentrations predicted at sites



**Figure 6.** CMAQ-predicted PM<sub>2.5</sub> concentrations on 28 February 2007 (LT) at the South DeKalb monitoring site with wind speed perturbations. Base case simulation results are also included.





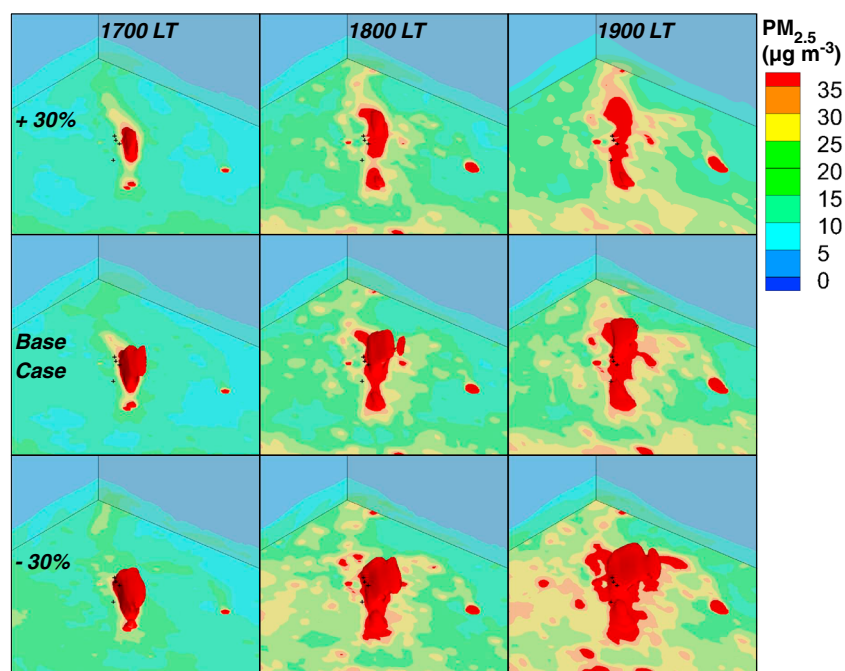
**Figure 7.** Maximum CMAQ-predicted PM<sub>2.5</sub> concentrations at the Confederate Ave., Jefferson St., South DeKalb, and McDonough monitoring sites with wind speed perturbations ranging from  $-50\%$  to  $+50\%$ .

within Atlanta increased by as much as 8 to 30% with perturbed wind fields, although remaining well below observed levels. However, the effect of the wind direction variations at each receptor may vary significantly. Figure 4 shows the change in predicted PM<sub>2.5</sub> concentrations relative to the base case simulation at different monitoring sites after applying a  $-5^\circ$  perturbation to wind direction. Although the responses are quite similar at the Confederate Ave. and Jefferson St. sites 8 km apart, appreciable differences exist between the sensitivities at these locations and South DeKalb, 7 km from Confederate Ave., where the maximum change in predicted PM<sub>2.5</sub> concentration is significantly lower. At McDonough, approximately 40 km closer to the fires, the response is larger and, compared to the Atlanta sites, appears to reflect a 2 h advance consistent with expected differences in transport time.

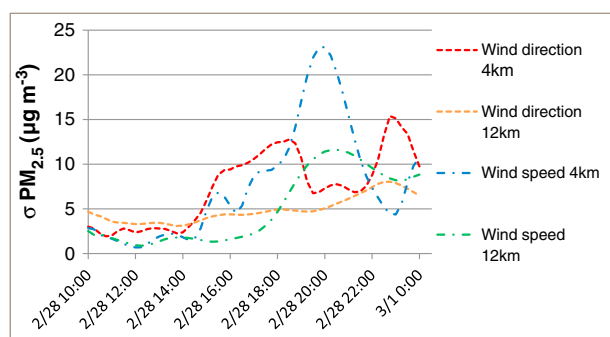
[17] The influence of wind direction on air quality modeling results can be observed in Figure 5 which compares ground-level PM<sub>2.5</sub> concentration predictions after perturbing wind direction by  $-5^\circ$  and  $+5^\circ$ . The figure shows how a  $10^\circ$  difference in wind direction can completely change a smoke plume's predicted impact at downwind receptors. Within this  $10^\circ$  wind direction variation range, predicted PM<sub>2.5</sub> concentrations at Atlanta may vary by more than  $30 \mu\text{g m}^{-3}$ . It is important to note that although errors in wind direction may partially explain the discrepancy between modeled and observed concentrations, simply inducing a directional adjustment on wind fields should not be considered a robust strategy to strengthen model performance. While it was possible to reduce the gap between observed and predicted peak PM<sub>2.5</sub> concentrations in Atlanta by modifying wind direction in meteorological inputs, perturbed wind fields decreased the root mean squared error (RMSE), estimated from the differences between modeled and observed values, only at Jefferson St. and McDonough. Still, the sensitivity analysis demonstrates that wind direction in meteorological inputs is a key element of air quality simulations attempting to replicate the impacts of fires and accurate wind directions are essential to produce realistic predictions.

#### 4.1.2. Wind Speed

[18] The methodology previously described in section 3.2 was also used to explore the sensitivity of CMAQ-predicted PM<sub>2.5</sub> concentrations to wind speed. Similar to the perturbations on wind direction, modified wind fields were produced by uniformly changing wind speeds by  $\pm 10\%$ ,  $\pm 20\%$ , and  $\pm 30\%$  across meteorological inputs. Figure S3 in the supporting information compares base case and perturbed wind fields. Large differences exist between predicted concentrations at downwind receptors under different modified fields.



**Figure 8.** Modeled pollution plumes on 28 February 2007 (LT) shown as three-dimensional isosurfaces bound by PM<sub>2.5</sub> concentration equal to  $35 \mu\text{g m}^{-3}$  for base case and simulations carried out with  $\pm 30\%$  perturbations to wind speed. Ground-level PM<sub>2.5</sub> concentrations ( $\mu\text{g m}^{-3}$ ) are also shown. Air quality monitoring sites are indicated by black markers.



**Figure 9.** Standard deviation of PM<sub>2.5</sub> concentration from CMAQ predictions on 28 February 2007 (LT) at Confederate Ave. for all simulations within the perturbation range applied to wind direction ( $\pm 5^\circ$ ,  $\pm 15^\circ$ ,  $\pm 30^\circ$ , and base case) and wind speed ( $\pm 10\%$ ,  $\pm 20\%$ , and  $\pm 30\%$ , and base case) under 4 km and 12 km horizontal grid resolutions.

In Figure 6, simulated PM<sub>2.5</sub> concentrations at the South DeKalb monitoring site are shown for each perturbation. A strong response to variations in wind speed is evident: at South DeKalb, a 30% decrease in wind speed elevated the peak PM<sub>2.5</sub> concentration by more than  $40 \mu\text{g m}^{-3}$ , an increase of nearly 75% with respect to the base case simulation. The responses are similar at all receptors considered; PM<sub>2.5</sub> concentrations significantly increased and experienced a growing delay with decreasing wind speeds. Unlike the response to wind direction, response to wind speed can be relatively linear. Figure 7 shows maximum PM<sub>2.5</sub> concentrations predicted by CMAQ at different downwind receptors as wind speed is perturbed from  $-50\%$  to  $+50\%$ . Response to wind speed is highly linear for negative perturbations but flattens out as magnitude is increased beyond a  $+10\%$  perturbation.

[19] Several factors contribute to the large differences in PM<sub>2.5</sub> concentration predictions obtained by applying different perturbations. Most importantly, changes to wind speed bring about significant differences in the dispersion of fire-related emissions. While larger wind speeds intensify advective dispersion, decreasing wind speed allows PM<sub>2.5</sub> emissions to accumulate within a smaller volume and reach higher concentrations. The effect wind speeds can have on smoke plume dispersion in Eulerian models is depicted in Figure 8. Here, smoke plumes are shown as three-dimensional isosurfaces bounded by PM<sub>2.5</sub> concentration equal to  $35 \mu\text{g m}^{-3}$ . As wind speed increases, dispersion of smoke occurs at a higher rate. The effect becomes more evident as winds strengthen with increasing altitude. Variations in wind speed also result in changes to the vertical winds within CMAQ. Generally, the perturbations to horizontal wind speeds yield a proportional increase or decrease in the vertical winds. This may further affect dispersion, enhancing it when wind speed is intensified and suppressing it when wind speed is reduced. In addition, wind speed perturbations may alter the trajectory traveled by the smoke plume and change the likelihood that it will directly impact a specific downwind receptor. Another factor leading to differences in predicted concentrations is the PBL height at the time of smoke arrival to the receptor. Finally, it is apparent that wind speed perturbations may also influence the dispersion of emissions from nonfire sources, including urban emissions. Therefore, the changes to PM<sub>2.5</sub> concentrations predicted under modified wind fields are due to the combined

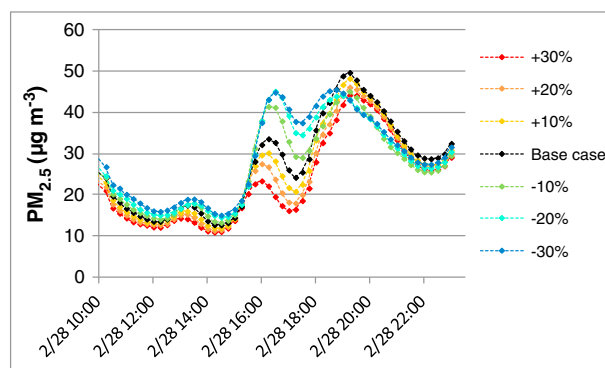
response of both fire-related impacts and the impacts from all other sources included in the simulation.

[20] Although errors related to wind speed cannot fully explain the difference between modeled and observed PM<sub>2.5</sub> concentrations, the sensitivity analyses suggest that uncertain wind speed estimates may play an important role in the underpredictions commonly associated with simulations attempting to replicate the air quality impacts of fires. In the smoke episode simulated for this study, reduced wind speeds led to higher peak PM<sub>2.5</sub> concentrations and prolonged air quality impacts, consistent with observations at downwind receptors. At the Atlanta locations considered, a 30% decrease in wind speed significantly improved model performance, reducing RMSE, estimated from the differences between modeled and observed PM<sub>2.5</sub> concentrations, at Confederate Ave., Jefferson St., and South DeKalb by 37%, 12%, and 36%, respectively. No gains in model performance were achieved at McDonough, GA, indicating that the prediction error at this location closer to the fires is more likely related to wind direction or the spatiotemporal allocation of fire emissions.

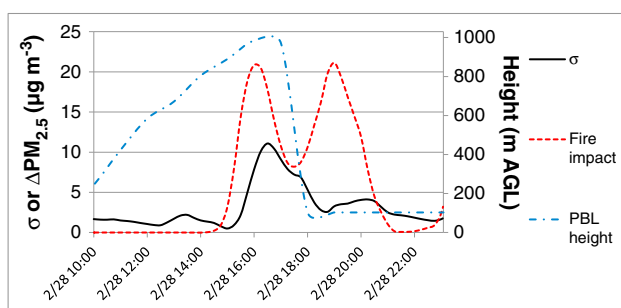
#### 4.1.3. Relation to Grid Resolution

[21] The importance of grid resolution in simulations attempting to replicate the air quality impacts of fires with chemical transport models was closely investigated using the base case considered for this study in Garcia-Menendez *et al.* [2010]. The analyses described therein showed that CMAQ-predicted PM<sub>2.5</sub> levels at sites downwind of fires are significantly affected by horizontal grid resolution of the model domain. In assessing the responsiveness of modeled concentrations to wind field inputs, it is important to consider the influence of model resolution on sensitivity estimates. Increased grid resolution can reduce numerical diffusion and produce better defined atmospheric plumes. Additionally, simulations carried out with coarser resolution become less sensitive to the spatial allocation of fire emissions on a gridded domain. This is especially true if emissions are allocated into a single coarse cell and concentration gradients are spatially smoothed immediately upon injection. Under these conditions, the sensitivities of air quality model predictions to uncertain wind fields may be greatly enhanced.

[22] To explore the relationship between grid resolution and the sensitivities of CMAQ-predicted PM<sub>2.5</sub> concentrations,



**Figure 10.** CMAQ-predicted PM<sub>2.5</sub> concentrations on 28 February 2007 (LT) at the Jefferson St. monitoring site under perturbed PBL heights. Base case simulation results are also included.



**Figure 11.** Standard deviation ( $\sigma$ ) of CMAQ-predicted PM<sub>2.5</sub> concentrations on 28 February 2007 (LT) for all simulations carried out under different PBL heights ( $\pm 10\%$ ,  $\pm 20\%$ , and  $\pm 30\%$ , and base case) and base case PBL height prediction at Confederate Ave. (right vertical axis). The estimated fire-related contribution to PM<sub>2.5</sub> concentration ( $\Delta PM_{2.5}$ ) is also included.

the Atlanta 2007 smoke episode was modeled under coarser 12 km horizontal grid resolution. Sensitivities to wind direction and speed were then evaluated by repeating the simulations under modified wind fields using the same perturbations described in sections 4.1.1 and 4.1.2. The analyses showed that simulated PM<sub>2.5</sub> levels at the downwind receptors considered were significantly less sensitive to wind field perturbations under coarser grid resolution. Figure 9 compares the standard deviation of predicted PM<sub>2.5</sub> concentrations at Confederate Ave. for all simulations carried out under perturbed wind fields using 12 km horizontal grid resolution to that of simulations using 4 km resolution, after fire-related emissions have begun. The values reflect the spread of CMAQ predictions within the perturbation range applied to wind direction ( $\pm 5^\circ$ ,  $\pm 15^\circ$ ,  $\pm 30^\circ$ , and base case) and wind speed ( $\pm 10\%$ ,  $\pm 20\%$ , and  $\pm 30\%$ , and base case). At Confederate Ave., the average standard deviation for PM<sub>2.5</sub> concentrations within both the wind direction and wind speed simulation sets decreases by approximately 35% when horizontal grid resolution is coarsened from 4 to 12 km. Maximum hourly standard deviations fall by nearly 50% when grid spacing is increased. The impact of coarser resolution is similar at other sites within the city of Atlanta (not shown); average standard deviation decreases by 25% and 38% at Jefferson St. and South DeKalb, respectively, while peak values drop by more than 40% at both locations. The effect is stronger at McDonough where reductions greater than 50% and 70% to average and maximum standard deviations, respectively, are observed after coarsening resolution. At this site, the enhanced impact of grid resolution is brought about by decreased diffusion at shorter range and how denser smoke plumes react to changes in winds.

[23] The differences between the sensitivities of PM<sub>2.5</sub> concentrations to wind fields using 4 and 12 km horizontal grid spacing demonstrate a strong connection between the potential impact of meteorological uncertainty and model resolution. As fire-related air quality simulations undertaken with Eulerian models move towards even finer levels of resolution, the sensitivity of predicted pollutant concentrations to wind fields can be expected to increase. Under such conditions, errors associated with meteorological inputs may strongly propagate to air quality predictions and offset some of the gains achieved from increased grid resolution.

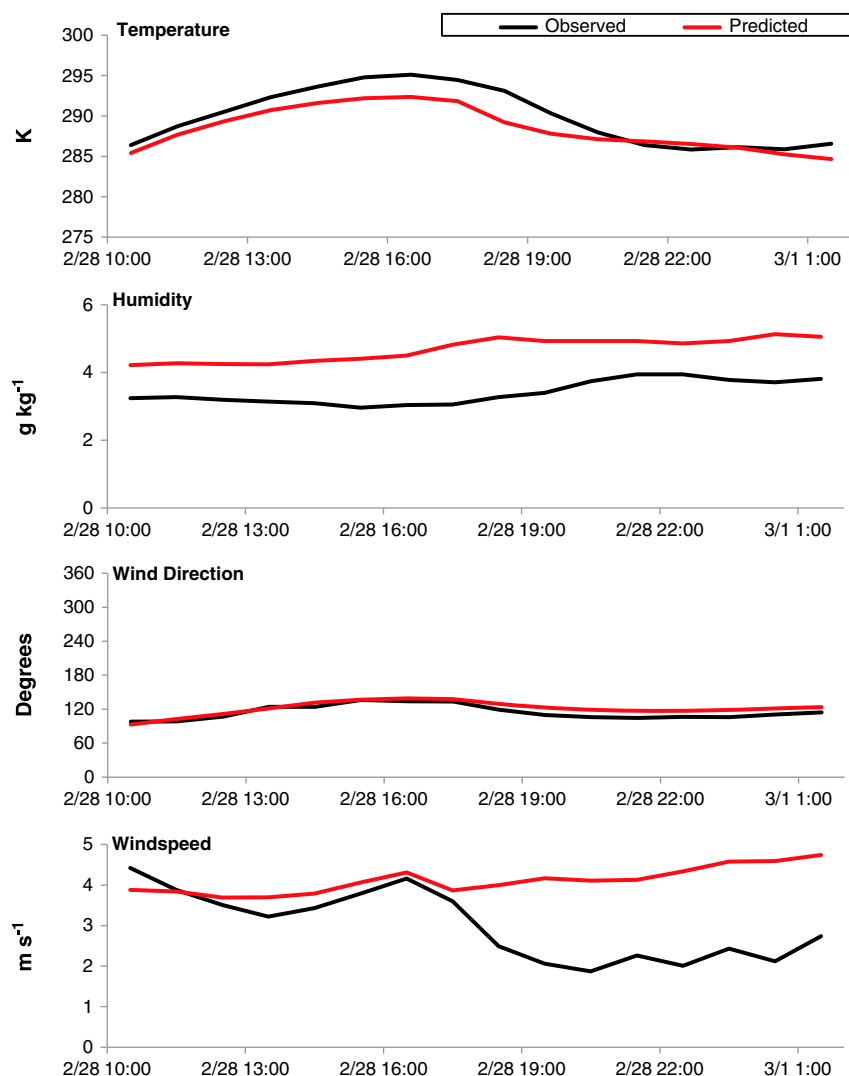
#### 4.1.4. Relation to PBL Height

[24] Winds are a major meteorological driver associated with fire-related air quality impacts and the focus of this study. However, PBL height is a fundamental parameter that shapes the turbulent atmospheric volume in which pollutants are readily dispersed. Previous analyses have identified the vertical allocation of fire-related emissions as a key element of smoke forecasting [Stein *et al.*, 2009]. In CMAQ 4.5, the similarity theory option was used to parameterize eddy diffusivity according to the PBL data produced by meteorological models. PBL heights influence the wind flow used to transport fire-related emissions and may significantly affect the predictions of air quality models. However, large discrepancies between PBL heights estimated by different meteorological models and observational data have been reported [Vautard *et al.*, 2012]. Uncertainty in PBL height fields may propagate in model results and influence their sensitivity to winds.

[25] To explore the sensitivity of CMAQ-predicted PM<sub>2.5</sub> concentrations at downwind receptors to PBL height, the Atlanta 2007 smoke episode was simulated with modified meteorological inputs. Similar to the sensitivity analyses centered on wind fields, PBL heights produced by WRF were perturbed by  $\pm 10\%$ ,  $\pm 20\%$ , and  $\pm 30\%$  to evaluate the responsiveness of predicted PM<sub>2.5</sub> concentrations to these variations. Significant sensitivities to PBL heights were evident at all downwind receptors considered. Figure 10 shows modeled PM<sub>2.5</sub> concentrations at Jefferson St. for each simulation carried out under perturbed PBL heights. Initially, and for much of the simulation, PM<sub>2.5</sub> concentrations at all sites are inversely related to PBL height. However, the correlation is not permanently negative and reflects the continual interaction between PBL height, plume rise, and emissions transport. While lowering the PBL height constrains pollutants within to a smaller volume, therefore increasing ground-level concentrations, it may also allow a greater fraction of the fire emissions to reach the free troposphere and be transported above the PBL, reducing their impact on surface air quality. In Figure 11, the standard deviation of predicted PM<sub>2.5</sub> concentrations at Confederate Ave. is shown for all simulations carried out with different PBL height fields. Also included are the base case PBL height predicted by WRF at the site and the fire-related contribution to PM<sub>2.5</sub> concentration estimated by comparing the results of simulations with and without fire emissions. Figure 11 shows how the sensitivity of PM<sub>2.5</sub> concentrations to PBL height, reflected in the standard deviation, evolves throughout the episode. At Confederate Ave., the strongest sensitivity to PBL height

**Table 1.** Daily Performance Benchmarks for Air Quality Modeling Applications Suggested by Emery *et al.* [2001] and Episode-Mean Performance Metrics for the Base Case Meteorological Modeling

|                                   | Recommended Benchmark | Base Case Simulation |
|-----------------------------------|-----------------------|----------------------|
| Temperature Bias (K)              | $\pm 0.5$             | -0.6                 |
| Temperature Error (K)             | 2.0                   | 1.5                  |
| Mixing Ratio Bias (g/kg)          | $\pm 1.0$             | 1.0                  |
| Mixing Ratio Error (g/kg)         | 2.0                   | 1.0                  |
| Wind Direction Bias ( $^\circ$ )  | $\pm 10$              | 8.5                  |
| Wind Direction Error ( $^\circ$ ) | 30                    | 9.6                  |
| Wind Speed Bias ( $m s^{-1}$ )    | $\pm 0.5$             | 1.3                  |
| Wind Speed RMSE ( $m s^{-1}$ )    | 2                     | 2.1                  |



**Figure 12.** Mean observed and WRF-predicted ground-level temperature, humidity, wind direction, and wind speed over northern Georgia for 15 h starting at 1000 LT on 28 February 2007.

occurs at the confluence of elevated PBL height and large fire-attributable PM<sub>2.5</sub> impacts. Similarly, at all receptors considered (not shown), the variation among model predictions is greatest when fire-related emissions contribute significantly to PM<sub>2.5</sub> concentrations and their injection into the atmospheric boundary layer is most susceptible to changes in PBL height.

## 4.2. Wind Field and Meteorological Uncertainty

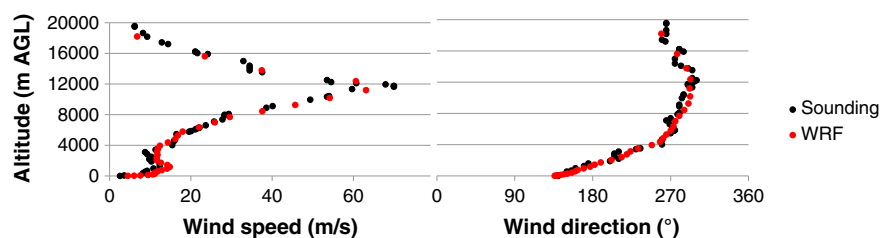
### 4.2.1. Ground-Level Observations and Model Comparison

[26] Wind fields generated by WRF were evaluated against surface-layer hourly observations from weather stations located within the base case modeling domain. Observations and predictions from 33 stations were spatially and temporally paired to calculate episode-mean performance metrics for key meteorological variables. Table 1 includes estimated statistical metrics as well as suggested performance benchmarks for meteorological models in air quality modeling applications [Emery *et al.*, 2001]. For this simulation, the metrics generally reflect adequate performance by WRF. Additionally, the statistics are comparable to those reported by annual

evaluations of meteorological model performance in air quality modeling applications [Gilliam and Pleim, 2010; Gilliam *et al.*, 2006; Hu *et al.*, 2010]. However, the evaluation does expose a significant positive bias in ground-level wind speed predictions that is outside the recommended range.

[27] To focus on the meteorology driving fire emissions transport, observations and predictions were compared spatially and temporally within a 150 km × 150 km window centered over plume trajectories for the Atlanta 2007 smoke episode. The window includes hourly weather observations from a subset of 12 weather stations. Figure 12 compares mean predicted and observed temperature, humidity, wind direction, and wind speed within the evaluation window from the initial release of fire-related emissions until the end of the simulation. During fire emissions transport, the mean bias and error in temperature predictions compared to observation were −1.5 K and 1.6 K, respectively. Simulated humidity displayed a consistent positive bias equal to 1.3 g kg<sup>-1</sup>. The uncertainties associated with predicted wind fields are of greater significance to simulations attempting to replicate the impacts of fires on downwind PM<sub>2.5</sub> concentrations. The mean





**Figure 13.** Wind speed and direction predicted by WRF (red) upper air observations (black) from the rawinsonde launched from Peachtree City, GA at 1900 LT on 28 February 2007.

bias and error in wind direction predictions with respect to observations were  $+5.8^\circ$  and  $6.9^\circ$ , respectively. Nevertheless, the maximum hourly wind direction error is nearly  $15^\circ$ . During the episode, the mean bias and error in simulated wind speeds were  $+1.1 \text{ m s}^{-1}$  and  $1.2 \text{ m s}^{-1}$ , respectively. Wind speed predictions closely agree with observations during the first half of the episode and exhibit a positive bias of approximately  $2 \text{ m s}^{-1}$  thereafter. Similarly, discrepancies between surface-layer observations and WRF-predicted wind speed and direction have been reported by other studies [Borge *et al.*, 2008; de Foy *et al.*, 2009]. The uncertainties in WRF-generated surface-layer winds, especially wind speeds, are relevant to air quality modeling involving smoke plume transport given the large sensitivities to variations in winds described in sections 4.1.1 and 4.1.2. However, fire-related emissions are largely transported above the surface-layer and a stronger response to wind flow at higher altitude should be expected.

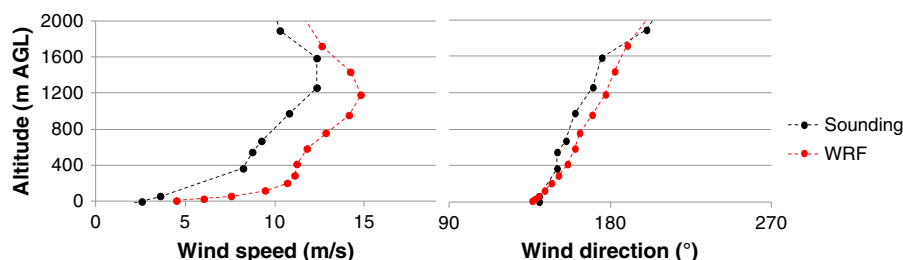
#### 4.2.2. Atmospheric Soundings and Model Comparison

[28] Atmospheric soundings provide an opportunity to evaluate upper air meteorological predictions. Within the simulation domain used for this study, sounding balloons were launched every 12 h from Peachtree City, GA, approximately 45 km southeast of Atlanta. Sounding data were paired spatially and temporally with WRF predictions to assess uncertainty in the meteorological fields used to drive the simulations. Figure 13 compares wind speed and wind direction data from the rawinsonde launched at 1900 LT on 28 February 2007 with WRF-predicted wind fields. This sounding provides the closest available record of upper air measurements, spatially and temporally, to the peak PM<sub>2.5</sub> concentrations observed in Atlanta during the 2007 smoke episode. Across the full vertical modeling domain, WRF-predicted wind fields display good agreement with the sounding observations. Overall, wind speed predictions compared to observations show a  $+0.5 \text{ m s}^{-1}$  mean bias, a 7.4% mean normalized bias, and a mean normalized error

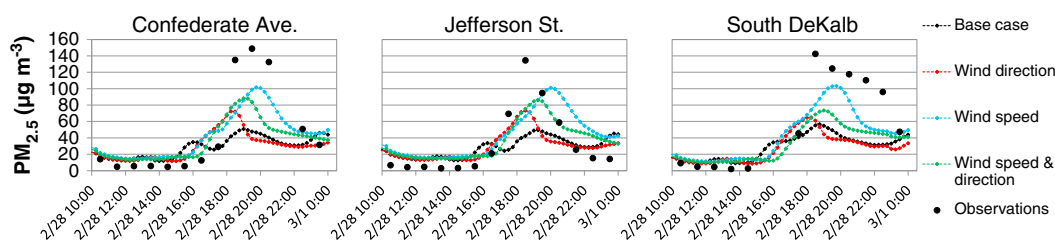
equal to 14.1%. Model performance is similarly strong for wind direction. When compared to sounding data across the vertical plane, WRF wind direction predictions show a mean bias of  $+1.82^\circ$  and a mean error equal to  $5.4^\circ$ .

[29] However, fire emissions transport only occurs within a fraction of the modeling domain. In our base case simulation, fire-related emissions are injected into the modeling domain up to 1300 m above ground level, and pollutant concentrations at downwind receptors are most sensitive to emissions released and transported within the PBL. Likewise, other studies suggest that low and middle PBL winds dominate the local and regional transport of fire-related emissions [Stohl, 1998]. Figure 14 focuses on the lower domain and again compares WRF-predicted winds to sounding observations. It becomes clear that at lower altitudes, where wind flow drives the transport of fire-related emissions, the model significantly overpredicts wind velocity. A bias in wind direction persists in the lower layers as well. Within the lowest 1500 m of the modeling domain, WRF forecasts overestimate wind speed by 40.2% with respect to sounding observations and display a  $6.8^\circ$  directional bias.

[30] The discrepancies between sounding data and WRF-generated wind fields demonstrate that significant uncertainties exist in the meteorological inputs used to drive air quality modeling. During the full 36 h CMAQ base case simulation, modeled wind speed and direction can differ significantly with concurrent upper air soundings within the lower levels of the modeling domain. Wind speeds near the surface are consistently overestimated by WRF. Discrepancies between predicted and observed wind directions are mostly lower than  $10^\circ$  and do not reflect a clear model bias for this episode. Similarly, other comparisons of WRF-predicted boundary layer winds speed and direction to wind profiler and aircraft observations have identified significant discrepancies [Gilliam and Pleim, 2010]. Furthermore, systematic positive biases for boundary-layer wind speed were also revealed in a collective evaluation of mesoscale meteorological models within the framework of the Air Quality Model Evaluation Initiative [Vautard *et al.*, 2012].



**Figure 14.** WRF-predicted wind speed and direction and observations from the rawinsonde launched from Peachtree City, GA at 1900 LT on 28 February 2007 for lower 2000 m of the atmosphere.



**Figure 15.** PM<sub>2.5</sub> concentration predictions on 28 February 2007 (LT) at Atlanta monitoring sites for base case CMAQ simulation, simulations with perturbed wind speed ( $-27\%$ ) and wind direction ( $-6.8^\circ$ ), and simulation with combined wind speed and wind direction perturbations. Monitoring station observations are also included.

### 4.3. Wind-Associated Error in PM<sub>2.5</sub> Predictions

[31] Meteorological fields are a key driver in air quality modeling. Errors associated with meteorological inputs propagate through air quality models and affect the accuracy of pollutant concentration predictions. Therefore, it is essential to evaluate the extent to which the performance of air quality models may be limited by uncertain meteorological input data. The process entails (1) determining the output variables most relevant to the modeling application, (2) identifying the input variables that significantly influence the values of the outputs of interest, (3) assessing the range of uncertainty in these model inputs, and (4) quantifying the sensitivity of output variables to input variable perturbations within their uncertainty range. In simulations attempting to replicate the impacts of wildland fires on air quality, ground-level pollutant concentrations at downwind locations are the output variables of greatest interest. Furthermore, in this study, we focus on PM<sub>2.5</sub>, the atmospheric pollutant most commonly associated with fire-related air quality impacts. Typically, a few input variables control the value of specific model outputs. For air quality simulations involving wildland fires, wind inputs are clearly among the variables dominating predicted PM<sub>2.5</sub> concentration. Here, uncertainties in wind inputs were explored by comparing meteorological predictions and observations. Finally, brute-force sensitivity analyses were used to determine the potential response of modeled PM<sub>2.5</sub> concentrations to errors in wind field inputs.

[32] The sensitivity analyses described in section 4.1 show that CMAQ-predicted PM<sub>2.5</sub> concentrations could respond strongly to wind field variations well within their uncertainty bounds. Previous studies have compared pollutant trajectories projected from wind profiler observations and model predictions and have revealed that large deviations (100–200 km) may develop over a 24 h period within the lower 1000 m of the atmosphere [Gilliam *et al.*, 2006; Godowitch *et al.*, 2011]. These transport errors, largely attributed to wind speed differences, could significantly influence air quality predictions. In this study's base case simulation, we revealed a positive bias in wind speed predictions with respect to both ground-level and upper air observations. The comparisons to weather data also revealed errors in wind direction predictions, generally smaller than  $10^\circ$ . The uncertainties in weather forecasts should not come as a surprise. However, it is clear that even small errors in wind flow can lead to large variations in PM<sub>2.5</sub> concentration predictions. Across the lowest 1500 m of the modeling domain, wind speed in meteorological inputs would need an average

reduction of 27% to match observed values from the available atmospheric sounding. Likewise, an average adjustment of  $-6.8^\circ$  to wind direction is needed to equate predicted and observed values across the same vertical range.

[33] Figure 15 compares base case PM<sub>2.5</sub> concentration predictions at Atlanta to results from simulations in which wind speed was systematically reduced by 27% and wind direction was uniformly modified by  $-6.8^\circ$ . The differences among predictions exemplify how errors associated with wind fields in meteorological inputs propagate into the output fields thereby limiting model performance. The reduction in wind speed increased the maximum predicted PM<sub>2.5</sub> concentrations within Atlanta by  $47\text{--}52\text{ }\mu\text{g m}^{-3}$  (82–103%) and delayed peak concentrations by approximately 1 h. Modifying wind direction resulted in earlier peak PM<sub>2.5</sub> concentrations and an  $8\text{--}24\text{ }\mu\text{g m}^{-3}$  (15–47%) increase to maximum predicted pollution levels. Additionally, Figure 15 shows the combined effect of simultaneously modifying wind speed and wind direction in meteorological input fields. The impacts of different perturbations on simulated concentrations are not additive, but rather each wind field produces a unique solution. Under specific conditions, the influence of errors associated with either wind speed or wind direction can dominate concentration estimates. Nevertheless, the analyses show that CMAQ-predicted PM<sub>2.5</sub> concentrations in simulations attempting to replicate the air quality impacts of fires may carry normalized errors as high as 100% due to uncertain wind inputs.

## 5. Conclusions

[34] The results of this study show that air quality estimates from chemical transport models attempting to replicate the impacts of wildland fires are extremely sensitive to meteorological fields. For such an application, model performance largely depends on the accuracy of wind inputs. More importantly, simulated pollutant concentrations displayed large sensitivities to variations in wind fields well within the uncertainty range of numerical weather prediction. Errors associated with wind data may largely account for considerable discrepancies frequently observed between monitored air quality levels and predicted PM<sub>2.5</sub> concentrations. Overestimated wind speeds in the lower atmosphere may be especially significant.

[35] However, shortcomings in model performance can only be partially explained by meteorology. Additional parameters and inputs have been identified as sources of error. Fire-related emissions remain uncertain, especially for

precursors of secondary organic aerosol. The spatiotemporal allocation of fire emissions on gridded domains may also impact model predictions. The significance of grid resolution in air quality simulations involving wildland fires was ascertained in Garcia-Menendez et al. [2010]. However, in the episode modeled for this study, the influence of uncertainty in wind inputs on concentration predictions substantially outweighed the effect all other sources of error identified, including uncertain emission rates. This suggests that fire-related simulations with chemical transport models are limited by the performance of existing numerical weather prediction systems. Additionally, as air quality modeling moves towards finer grid resolution, errors associated with meteorological inputs can be expected to constrain model accuracy even further.

[36] The response of PM<sub>2.5</sub> concentration predictions to wind flow perturbations signals a need to include meteorological inputs in any strategy designed to improve fire-related air quality simulations. Furthermore, it is important to recognize the limitations inherent to weather forecasts in the context of air quality modeling. Uncertain wind fields are an intrinsic component of numerical weather prediction and mitigating errors in short-term and small-scale wind forecasts produced by existing models is a challenging task. Concerns about the ability of meteorological models to capture intraday wind variations have been previously raised [Hogrefe et al., 2001]. Additionally, substantial variability exists in meteorological predictions from different models and different configurations of the same model [Vautard et al., 2012]. In light of this, air quality forecasts predicting the impact of fires on air quality produced by atmospheric chemistry and transport models must be considered substantially uncertain. These uncertainties must be considered when air quality modeling is used to steer fire management decision making.

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