Simulating smoke transport from wildland fires with a regional-scale air quality model: Sensitivity to spatiotemporal allocation of fire emissions

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A B S T R A C T
Air quality forecasts generated with chemical transport models can provide valuable information about the potential impacts of fires on pollutant levels. However, significant uncertainties are associated with fire-related emission estimates as well as their distribution on gridded modeling domains. In this study, we explore the sensitivity of fine particulate matter concentrations predicted by a regional-scale air quality model to the spatial and temporal allocation of fire emissions. The assessment was completed by simulating a fire-related smoke episode in which air quality throughout the Atlanta metropolitan area was affected on February 28, 2007. Sensitivity analyses were carried out to evaluate the significance of emission distribution among the model’s vertical layers, along the horizontal plane, and into hourly inputs. Predicted PM$_{2.5}$ concentrations were highly sensitive to emission injection altitude relative to planetary boundary layer height. Simulations were also responsive to the horizontal allocation of fire emissions and their distribution into single or multiple grid cells. Additionally, modeled concentrations were greatly sensitive to the temporal distribution of fire-related emissions. The analyses demonstrate that, in addition to adequate estimates of emitted mass, successfully modeling the impacts of fires on air quality depends on an accurate spatiotemporal allocation of emissions.

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1. Introduction

Wildland fires, including wildfires and prescribed burns, can significantly increase the air pollution burden at urban locations across extensive regions downwind (Amiridis et al., 2012; K.H. Lee et al., 2005; Miranda et al., 2009; Phuleria et al., 2005; Witham and Manning, 2007). The effect of fires on fine particulate matter (PM$_{2.5}$) concentrations deserves special attention; fire-related impacts on air pollutant levels are strongest for PM$_{2.5}$ and may lead to unhealthy air quality (Delfino et al., 2009; Henderson et al., 2011; Rappold et al., 2011) and reduced visibility (Park et al., 2006; Wise, 2008). Furthermore, fires can account for an important fraction of PM$_{2.5}$ pollution (Mueller and Mallard, 2011; Park et al., 2007).

Air quality forecasts produced with numerical models can provide valuable information to environmental managers about the potential impacts of fires. Eulerian chemical transport models (CTMs) are an attractive option to simulate the dispersion and transformation of fire emissions. Multiscale capabilities in current CTMs allow the transition of fire-related air pollution from local scales into larger regional scales to be reproduced. Complex atmospheric transformations affecting fire emissions may be modeled through state-of-the-science representations of chemical and physical processes. Additionally, comprehensive emissions inventories and weather inputs allow CTMs to simulate the interactions of pollutants with detailed meteorological fields and background atmospheres.

Previous studies have attempted to replicate the air quality impacts of fires using CTMs (Chen et al., 2008; Hodzic et al., 2007; Junquera et al., 2005; Konovalov et al., 2011; Zeng et al., 2008). Only a few of these simulations sought to replicate distinct smoke plumes and evaluated model predictions against measured or satellite-derived pollutant levels. Such evaluations have reported mixed results when aiming to reproduce observed particle loads downwind of specific fires. A considerable amount of research investigating the effects of wildland fires on air pollution has focused on determining fire-related emissions and emission factors (Akagi et al., 2011; S. Lee et al., 2005; Wiedinmyer et al., 2006). However, the distribution of fire emissions along space and time on gridded modeling domains is also subject to significant uncertainty (Tian, 2006). Beyond the magnitude of emissions, the methodologies applied to introduce fire emissions into air quality simulations must be assessed.

Sensitivity analyses can be used to quantify the responsiveness of models to specific inputs or parameters. By doing so, they weight the relative importance of each input variable to select outputs and provide key information to improve model performance. Here, we explore the sensitivity of PM$_{2.5}$ concentrations simulated by a regional-scale CTM to the spatial and temporal allocation of fire emissions during a large fire-related smoke episode. Sensitivity analyses were performed to evaluate the significance of plume rise approximations and distribution

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of fire emissions among a model’s vertical layers. The implications of emission allocation along the horizontal plane were also explored by assessing the effect of treating fires as single-cell point sources or distributing emissions into multiple cells. Additionally, a sensitivity analysis of simulated concentrations to the temporal partitioning of fire emissions into hourly inputs is presented. The results of this study weigh the potential benefits of better characterizing fire emissions in CTMs beyond emission strength.

2. Methods

2.1. Air quality modeling framework

Numerical air quality modeling was done with the U.S. Environmental Protection Agency’s Community Multi-scale Air Quality modeling system (CMAQ) (version 4.5, http://www.cmaq-model.org/). CMAQ is a third-generation emissions-based system widely applied for regulatory analysis and atmospheric research. CMAQ includes state-of-the-science parameterizations of physical and chemical processes that affect gaseous and particulate airborne pollution (Byun and Schere, 2006). In addition, CMAQ’s multiscale capabilities allow simulations to cover multiple scales from local to continental.

Meteorological fields were produced with the Weather Research and Forecasting model (WRF version 2.2, http://www.wrf-model.org/index.php). WRF simulations were carried out using 3 nested domains at 36, 12, and 4 km horizontal grid resolution. Analysis products from the North American Mesoscale model (nomads.ncdc.noaa.gov) were used to initialize weather simulations, constrain boundary conditions, and nudge meteorological fields at 6-hour intervals. Additional details about the WRF configuration are available in Garcia-Menendez et al. (2013).

Pollutant emission rates for non-fire sources were prepared through the Sparse Matrix Operator Kernel Emissions modeling system (SMOKE version 2.1, http://www.smoke-model.org/index.cfm) using emissions projected from a 2002 “typical year” emissions inventory (MACTEC, 2005). Fire-related emissions were estimated with the Fire Emission Production Simulator (FEPS version 1.1.0, http://www.fs.fed.us/pnw/fera/feps/). FEPS can be used to model hourly emissions and heat release from prescribed burns and wildfires involving a variety of fuel types.

In all CMAQ simulations, modeling domains were divided into 34 sigma-pressure vertical layers. Layer thickness increased from approximately 20 m at the surface to over 3 km at the domain’s upper edge approximately 20 km above. The first 1000 m of the atmosphere were contained within the 10 lowest layers. The vertical distribution of fire emissions was derived from plume rise estimates from the Daysmoke model (Achtemeier et al., 2011). Analogous to the WRF simulations, CMAQ air quality modeling was performed using 3 nested grids. Coarser-resolution simulations were used to define initial and boundary conditions for fine-resolution modeling. All sensitivity analyses relied on simulations performed at 4 km resolution.

2.2. Base case simulation

Fire-related smoke severely impacted air quality across metro Atlanta on February 28, 2007. The increase in pollutant concentrations is believed to have been caused by two prescribed burns roughly 80 km southeast of Atlanta at the Oconee National Forest and Piedmont National Wildlife Refuge (henceforth referred to as Oconee and Piedmont). Approximately 12 km² of wildland was affected by these fires. Hourly PM$_{2.5}$ concentrations observed throughout Atlanta escalated to around 150 µg m$^{-3}$ a few hours after ignition. Fig. 1 shows the locations of the fires and air quality monitoring stations considered in this study.

This episode has been modeled with CMAQ for several studies. Hu et al. (2008) compared an air quality forecast executed with preburn information to a series of “hindcasts” that incorporated additional details about the fires and observed meteorology. Liu et al. (2009) analyzed smoke transport from the burns and compared simulated trajectories to satellite observations. In Garcia-Menendez et al. (2010), an adaptive grid version of CMAQ capable of dynamically refining grid resolution was used to simulate the smoke plume. In Garcia-Menendez et al. (2013), the sensitivities of predicted PM$_{2.5}$ concentrations to uncertainty in meteorological inputs during the episode were explored.

Fig. 2 shows hourly PM$_{2.5}$ emissions estimated by FEPS for each burn. FEPS requires approximations of burn area, fuel consumption, and emission factors. Reported uncertainties for similar bottom-up estimates of PM$_{2.5}$ emissions from prescribed fires in the southeastern U.S. range from 15% to 50% (Odman, 2011; Tian, 2006). For instance, PM$_{2.5}$ emissions from a series of prescribed burns in northern Florida were approximated in a recent study using the same approach applied here and found to be underestimated by 15% with respect to field measurements (Odman, 2012). Hourly plume structures simulated by Daysmoke were used to distribute fire emissions among the vertical layers in CMAQ. Fig. 3 shows PM$_{2.5}$ injected into each layer from the Oconee and Piedmont fires for the entire simulation. Generally, upper layer emissions correspond to flaming combustion, while emissions distributed closer to the surface belong to the fire’s smoldering phase.

![Fig. 1. Location of Oconee and Piedmont fires, and Confederate Ave. (CFA), South DeKalb (SDK), Jefferson St. (JFS), and McDonough (MCD) air quality monitoring stations.](image1)

![Fig. 2. Hourly PM$_{2.5}$ emissions for the Oconee and Piedmont fires on February 28, 2007 (LT).](image2)
2.3. Sensitivity analyses

Sensitivities of CMAQ-modeled concentrations to fire emissions were quantified by calculating the difference between two simulations in which a parameter was perturbed,

$$s_x = \frac{C_{x+\Delta x} - C_{x-\Delta x}}{2\Delta x},$$  \hspace{1cm} (1)

where $s_x$ is the first-order sensitivity coefficient of concentration $C$ in response to parameter $x$, and $C_{x+\Delta x}$ and $C_{x-\Delta x}$ are the concentrations resulting from simulations under $+\Delta x$ and $-\Delta x$ perturbations to $x$. These sensitivity estimates, also known as “brute-force” sensitivities, can be applied to any simulated variable and model parameter or input (Hwang et al., 1997). In this work, sensitivity analyses were used to quantify the response of modeled PM$_{2.5}$ concentrations to variations in the temporal and spatial allocation of fire emissions. Each sensitivity estimate required two additional simulations beyond the base case. With the exception of fire-related emissions, model configuration and inputs in the sensitivity runs remained identical to those used in the base-case simulation. For sensitivities that reflect the response to emissions from a specific grid cell, vertical layer, or period of time, only emissions within that subset were perturbed.

Using the brute-force method to estimate sensitivities of modeled concentrations and project air quality impacts entails several considerations. Brute-force sensitivity estimates may be heavily influenced by numerical errors if excessively small perturbations are used (Hakami et al., 2004). The ability of sensitivity coefficients estimated by Eq. (1) to replicate response to larger or smaller perturbations depends on the response’s linearity. For many primary pollutants, the response of atmospheric concentrations to emission perturbations can be expected to be mostly linear (Cohan et al., 2005). Previous sensitivity analyses using CTMs have in fact shown a nearly linear source–receptor relationship for emissions (Koo et al., 2009).

Although most atmospheric aerosol-phase processes included in CMAQ are linear, some, such as thermodynamic aerosol interactions, cloud processes, and secondary aerosol formation, are not (Napelenok et al., 2006). In this study, the analyses of PM$_{2.5}$ concentration sensitivity to fire emissions focus on primary particle emissions. While secondary formation may contribute to fire-related PM$_{2.5}$, most of the impacts are attributable to primary emissions (Tian et al., 2009). Furthermore, although fire-related PM$_{2.5}$ impacts may not be entirely linear, the response to fire emissions in air quality models commonly is (Liu et al., 2009; Tian et al., 2008). Limited information about fire-related emissions of secondary aerosol precursors and their non-linear transformations frequently constrain smoke simulations to primary emissions and linear response. Additionally, PM$_{2.5}$ sensitivity estimates can be scaled to other primary pollutants and provide information about the dispersion-related response of all species.

3. Results and discussion

3.1. Base case model performance

CMAQ performance during the base-case simulation was evaluated by comparing predicted PM$_{2.5}$ concentrations to concurrent observations at air quality monitoring stations downwind of the fires where large increases to PM$_{2.5}$ levels were recorded during the smoke episode. Sites used for evaluation belong to the Georgia Department of Natural Resources (Confederate Ave., South DeKalb, and McDonough stations) and Southeastern Aerosol Research and Characterization (Jefferson St. station) networks. A visualization of the smoke plume simulated by CMAQ is shown in Fig. 4a.

Fig. 4b compares modeled and observed PM$_{2.5}$ concentrations at the Jefferson St. monitoring station in downtown Atlanta. A large underprediction in simulated peak PM$_{2.5}$ concentrations compared to measurements was evident. Similarly, CMAQ-estimated PM$_{2.5}$ concentrations were lower than observations at all monitoring sites significantly impacted by smoke. At sites within the city of Atlanta (Confederate Ave., Jefferson St., and South DeKalb) CMAQ underestimated maximum observed 1-hour average PM$_{2.5}$ concentrations by 58–67%. For these locations, the model’s mean fractional error ($2|C_{\text{modeled}} - C_{\text{observed}}|/(C_{\text{observed}} + C_{\text{modeled}})$) ranged from 64% to 73% during the 8-hour interval with the highest observed PM$_{2.5}$. However, the simulation did result in relatively well-timed hits at downwind receptors within Atlanta and produced a reasonable plume trajectory. At the McDonough station, about halfway between Atlanta and the prescribed burns, CMAQ underestimated the maximum observed PM$_{2.5}$ concentration by 33%. Still, an 8-hour mean fractional error of 67% indicated that the simulated concentration increase at the site was poorly timed relative to observations.

Additional CMAQ performance metrics are included in García-Menéndez et al. (2010) for a similar simulation. Likewise, previous studies have reported CMAQ-modeled PM$_{2.5}$ concentrations below ground-based observations when attempting to simulate fire-related impacts (Liu et al., 2009; Strand et al., 2012). For instance, Yang et al. (2011) modeled a series of wildfires along the Georgia–Florida border and found that predicted PM$_{2.5}$ concentrations were far lower than observations even after increasing fire emissions by a factor of three. The analyses included in García-Menéndez et al. (2010) showed that increased horizontal grid resolution may substantially raise modeled concentrations; by applying an adaptive grid version of CMAQ that dynamically refined grid resolution at the smoke plumes, peak simulated PM$_{2.5}$ concentrations in Atlanta increased by up to 40%. In García-Menéndez et al. (2013), large sensitivities to meteorological inputs for PM$_{2.5}$ concentrations simulated during this episode were identified. The discrepancies between predictions and observations may be largely attributable to uncertainty in meteorological data, wind fields in particular. Multiple factors simultaneously contribute to
the underestimated fire impacts and are discussed in Section 4. Here our objective is to assess the contribution of uncertainty in the spatiotemporal allocation of fire emissions to this error.

3.2. Fire contributions to PM$_{2.5}$ concentrations

Fire contributions to simulated PM$_{2.5}$ concentrations were approximated using brute-force sensitivity estimates. Fire-related particle emissions were determined from PM$_{2.5}$ emission factors and speciated mostly as primary organic aerosol (90%) and primary elemental carbon (6%). For these species, no significant nonlinear transformations in the model were expected. In addition, simulated PM$_{2.5}$ concentrations in Atlanta did not show a significant response to fire-related emissions of NOx, SO$_2$ and volatile organic compounds, derived from FEPS estimates for PM$_{2.5}$ and CO. Linear response allows impacts and source contributions to be approximated as

$$C = C_0 + s_x \Delta x,$$

(2)

where $C_0$ is a base-case concentration and $C$ is the concentration after perturbation $\Delta x$. A nearly linear relationship between modeled concentrations and fire emissions was identified at all downwind receptors across perturbations to base-case fire emissions ranging from −50% to +50%. The inclusion of second-order sensitivity coefficients into response estimates only changed total PM$_{2.5}$ impacts by less than 2%. Additionally, the base case was simulated using a more recent version of CMAQ (version 4.7.1) with updated treatments of aerosol dynamics and chemistry. However, the underestimate of peak PM$_{2.5}$ levels during the episode persisted in the values predicted by the updated model, with maximum concentrations within Atlanta slightly lower than those simulated by CMAQ 4.5. A linear response to perturbations in fire emissions was still evident in the CMAQ 4.7.1 simulations, with no significant formation of secondary aerosol.

Fig. 5a shows the first-order sensitivity coefficient for PM$_{2.5}$ concentration response to fire emissions at South DeKalb during the episode. The coefficient quantifies change in modeled concentration per ton of fire-emitted PM$_{2.5}$ as a function of time. Estimates at each instant represent sensitivity to all prior PM$_{2.5}$ emissions (i.e. cumulative fire-emitted PM$_{2.5}$). Fire and non-fire contributions to simulated PM$_{2.5}$ concentrations at South DeKalb are shown in Fig. 5b. The non-fire contribution was estimated from a CMAQ simulation without Oconee and Piedmont fire emissions, while the fire contribution was calculated using first-order sensitivity coefficients. Fig. 5b also includes results from a simulation with all emission sources and shows that these concentrations closely matched the sum of the estimated fire and non-fire contributions. A significant fraction of the CMAQ-predicted PM$_{2.5}$ pollution was attributable to fires. At Atlanta sites, the fire-attributable PM$_{2.5}$ impact reached 20–31 µg m$^{-3}$ and contributed up to 56–67% of the total modeled PM$_{2.5}$. At McDonough, the maximum fire contribution to modeled PM$_{2.5}$ concentration was 78% and the maximum fire-related impact was 70 µg m$^{-3}$. Contributions from non-fire sources were also significant and displayed large variations, characteristic of the daily fluctuation in urban concentrations. The importance of non-fire contributions has been acknowledged in previous modeling efforts exploring

![Image](image-url)
the air quality impacts of wildland fires (Christopher et al., 2009; Yang et al., 2011).

Sensitivity coefficients were also used to approximate the increase to fire emissions that would match maximum simulated PM$_{2.5}$ concentrations and peak observations. Fig. 6 shows the effect, estimated with Eq. (2), of intensifying base-line fire emissions by a factor of 5.1 at Jefferson St. and 3.7 at South DeKalb. Overall, base-line fire emissions would have to be increased by a factor of 4–6 for CMAQ predictions to reach the highest observed concentrations within Atlanta. Increments of this magnitude suggest that underpredicted downwind impacts cannot be fully explained by underestimated fire emissions. The projections also indicated that while modeled maxima were generally well-timed relative to peak observations, important differences did exist between the evolution of the predicted impacts and observed PM$_{2.5}$ concentrations throughout the episode.

Sensitivities were also calculated for each prescribed burn and used to compare PM$_{2.5}$ contributions specific to the Oconee and Piedmont fires. Fig. 7a shows PM$_{2.5}$ impacts by fire at South DeKalb. Although contributions from both fires were significant, about 75% of the total fire-related PM$_{2.5}$ impact was attributable to the Oconee burn. The disparity is brought about by unequal emissions and differences in concentration sensitivities to emissions from each fire. Fig. 7b shows hourly first-order sensitivity coefficients for each burn. Larger emissions from the Oconee burn largely drove the PM$_{2.5}$ impacts. However, sensitivity coefficients can be significantly higher for Piedmont emissions. While the added impact of Oconee emissions was larger, on average each ton of PM$_{2.5}$ emitted by the Piedmont burn led to a greater increase in concentrations at downwind locations. Moreover, the timing of peak sensitivity coefficients for the Piedmont fire better agreed with maximum simulated and observed concentrations. The sensitivity coefficients for each fire differ due to dissimilarities in the way fire emissions are distributed spatially and temporally. The difference corroborates the idea that the allocation of fire emissions into hourly rates and grid cells may significantly influence predicted concentrations.

3.3. Horizontal allocation of fire emissions

Fires are commonly treated as point sources along the horizontal plane in episodic air quality simulations with CTMs. The assumption entails injecting fire emissions into a single horizontal grid cell or stack of cells, while ignoring details about burn area and fire spread. In the base-case simulation, emissions from each fire were horizontally allocated to a single stack of cells at the centroid of burned areas. Errors associated with this simplification grow as grid resolution is increased. The Oconee and Piedmont fires each consumed approximately 6.2 and 5.9 km$^2$ of wildland, an area roughly equivalent to a 2.5 km × 2.5 km square. On a 4 km grid, it is likely that each fire might have extended across multiple cells. Furthermore, fire locations may be uncertain. Information regarding fire evolution may be limited, especially for wildfires. Satellite-based methods used to determine fire location and size may introduce additional uncertainty (Giglio et al., 2006; Henderson et al., 2010). Still, satellite-derived information can be used to spatially refine coarse fire characterizations (Roy et al., 2007). In this section we assess the potential gains of more accurately pinpointing fires or distributing their emissions across multiple cells.

For the Oconee and Piedmont burns, sensitivity estimates were used to compare PM$_{2.5}$ concentration impacts at downwind receptors for all 4 km × 4 km grid cells adjacent to the cell into which fire emissions were originally injected. Fig. 8 shows the change in total Oconee and Piedmont fire contributions to PM$_{2.5}$ at Jefferson St., relative to the

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Fig. 6. Base-case and projected PM$_{2.5}$ concentrations along with monitoring site observations on February 28, 2007 (LT). Projections estimate the effect of increasing fire emissions by factors of 5.1 (Jefferson St.) and 3.7 (South DeKalb).

Fig. 7. (a) Contributions to modeled PM$_{2.5}$ concentrations at South DeKalb from Oconee and Piedmont fires on February 28, 2007 (LT). Non-fire contribution and base-case CMAQ predictions are also included. (b) First-order sensitivity coefficients for PM$_{2.5}$ concentration response to fire emissions from each fire at South DeKalb (left axis) and site observations (right axis).
base case, after relocating fire-related emissions into cells neighboring the emissions’ original location (center cell). Additionally, simulated peak PM$_{2.5}$ concentrations were compared to the base-case maximum (54 µg m$^{-3}$) across the nine cell area. Results for other sites are included in the supplementary information. It is clear that small changes to the horizontal allocation of fire emissions may significantly affect modeled PM$_{2.5}$ concentrations downwind. For the Atlanta sites considered, reallocation of emissions from the Oconee fire into a neighboring grid cell could have increased their total PM$_{2.5}$ impact at a specific receptor up to 28% or lowered it by as much as 20%. A single-cell shift in the horizontal allocation of Oconee emissions, which only account for a fraction of total PM$_{2.5}$, could also cause peak concentrations at these sites to escalate or fall by up to 20%. At McDonough, closer to the burns, the sensitivity of concentrations to the horizontal allocation of fire emissions was even larger.

Changes in total PM$_{2.5}$ impacts brought about by reallocating fire emissions did not necessarily correspond to changes in peak concentrations. For example, shifting Oconee emissions one cell northeast increased total fire-attributable PM$_{2.5}$ at Confederate Av. by 8%, but decreased the maximum simulated PM$_{2.5}$ concentration by 12%. Furthermore, the response may be different for nearby receptors; while the reallocation operation described above led to an 8% increase in the fire-related PM$_{2.5}$ impact at Confederate Av., it caused a concurrent 20% reduction at South DeKalb 7 km away. Significant differences exist between the magnitudes and patterns of PM$_{2.5}$ concentration response to equivalent changes in the horizontal distribution of Oconee and Piedmont fire emissions, as shown in Fig. 8. However, the sensitivities of CMAQ-predicted PM$_{2.5}$ concentrations to the horizontal allocation of Piedmont fire emissions were also large; a single-cell shift could change total PM$_{2.5}$ contribution and peak concentration at Atlanta sites by up to 35% and 9% respectively.

Additional uncertainty regarding the horizontal positioning of fire emissions stems from the plume rise representations applied to account for buoyancy. Here plume structure was modeled to distribute fire emissions across the domain’s vertical layers. Daysmoke, a subgrid scale dispersion model, was used to approximate plume rise as the vertical distribution of fire-related particulate matter at a fixed downwind distance after full plume development. For this episode, the vertical plume structure was calculated 10 km downwind of the fires but used to vertically distribute fire emissions at the source. To evaluate the implications of applying a downwind plume rise estimate at the original fire location, PM$_{2.5}$ impacts were compared for emissions injection into cells 10 km downwind of fires (i.e. two grid cells northwest). Again, it was clear that relocating fire emissions can have a significant effect on predicted concentrations; allocating emissions downwind of the fires changed the fire-attributable PM$_{2.5}$ impacts and maximum simulated concentrations at Atlanta sites by up to 15%.

### 3.4. Vertical allocation of fire emissions

Plume rise approximations are an important component of air quality simulations involving buoyant emissions. As previously discussed, when fires are included in grid cells, their emissions must be distributed among the domain’s vertical layers. Frequently, vertical distribution profiles are determined from simplified theoretical or empirical plume rise approximations (Hodzic et al., 2007; Junquera et al., 2005). Fire emissions processors (e.g. FEPS) or subgrid-scale models may provide hourly maximum and minimum plume height estimates (Freitas et al., 2007; Sessions et al., 2011). Emissions can then be uniformly distributed among vertical layers from the maximum plume height down to the minimum height or ground. Fire emissions have also simply been homogeneously distributed within the planetary boundary layer (PBL) or below a fixed altitude (Hu et al., 2008; Yang et al., 2011). Alternatively, Lagrangian particle models can produce more realistic vertical plume structures that may be used to vertically allocate fire emissions on grid cells or even at the plume core but used for prescribed burns. To evaluate the influence of vertical allocation of fire emissions, the sensitivities of CMAQ-predicted PM$_{2.5}$ concentrations to fire emissions injected into each vertical layer were computed. Fig. 9 shows estimated fire contributions to PM$_{2.5}$ concentration at South DeKalb by vertical layer. The contribution from non-fire sources, determined from a simulation without fire emissions, and base-case CMAQ concentrations are also included. In the base-case simulation emissions were distributed across the lowest 11 layers. The largest fire contributions came from layers 8–10, accounting for over 65% of the fire-related impact on PM$_{2.5}$ concentrations. Recall that these layers received the largest fractions of fire emissions (Fig. 3).

Since layer-specific contributions largely depend on the amount of emissions injected into each layer, sensitivity estimates, which quantify
the response of concentration predictions per unit of emitted mass, are of greater relevance in assessing the significance of vertical profiles in air quality simulations. The sensitivities of PM<sub>2.5</sub> concentrations to fire emissions varied significantly between different vertical layers. Two distinct components of emissions in a vertical layer are responsible for the differences in sensitivities: injection altitude and emissions timing. If time-varying vertical perturbations are applied, simulated concentrations may be more responsive to emissions from a specific vertical layer due to the timing of injection rather than layer altitude. To isolate the influence of spatial or temporal allocation in brute-force sensitivity calculations, one component should be perturbed at a time. A constant vertical emissions profile was used to remove the temporal variability between layers. This enabled a true assessment of the sensitivity of modeled PM<sub>2.5</sub> concentrations to injection height, by equally splitting fire emissions into all layers considered throughout the episode. By allocating the same hourly fire emissions to each vertical layer, a fair comparison of their respective impacts can be made. Fig. 10 shows PM<sub>2.5</sub> concentration sensitivities to fire emissions by vertical layer at South DeKalb after applying a constant and layer-uniform vertical distribution to fire emissions across the lower 16 layers. The results indicate that after removing temporal variability from fire emissions, the sensitivities were similar for all vertical layers below layer 10. Sensitivity to layer 10 emissions was significantly lower and modeled PM<sub>2.5</sub> concentrations were not responsive at all to emissions injected above layer 10 or approximately 1000 m. The same conclusions can be drawn from sensitivity estimates at the other downwind sites.

The analysis reveals that for this episode CMAQ-predicted PM<sub>2.5</sub> concentrations were not overly sensitive to the vertical distribution of fire emissions, but rather only to whether emissions are injected above or below a specific altitude. This can be explained by analyzing the evolution of PBL height in the meteorological data. Fig. 11 shows WRF-predicted PBL height during the episode at the Oconee fire location along with full-layer heights for the 11 lowest vertical layers. In Section 3.5 below, we demonstrate that simulated PM<sub>2.5</sub> concentrations at South DeKalb were mostly sensitive to fire emissions released between 12:00 and 16:00 LT. During this time frame the PBL partially extended into layer 10 for only a fraction of the time and did not reach layers above. This indicates that modeled PM<sub>2.5</sub> concentrations responded similarly to all fire emissions injected within the PBL and were not affected by emissions released into the free atmosphere. Previous studies have reported similar findings. Yang et al. (2011) conclude that modifying the vertical distribution of fire emissions did not significantly affect CMAQ performance in their simulations. Sensitivity analyses performed on the National Oceanic and Atmospheric Administration’s Smoke Forecasting System determined that model effectiveness is greatly dependent on accurately determining whether smoke injection height occurred within or above the PBL (Stein et al., 2009). Although Liu et al. (2008) assert that PM<sub>2.5</sub> predictions from CMAQ are highly sensitive to plume rise approximations, differences in concentrations are most evident between their simulations with emissions distributed within the PBL and that with injection at much higher altitudes.

3.5. Temporal allocation of fire emissions

In addition to uncertainties related to the spatial allocation of fire emissions on gridded domains, uncertainty associated with the temporal distribution of emissions may affect an air quality model’s ability to simulate the impacts of fires. Emissions are generally input into CTMs as hourly rates. Similarly, fire emissions processors may provide daily or hourly estimates. However, partitioning of fire emissions into hourly rates may be complicated by limited information on starting time, duration, spread and evolution.

In this study, fire emission rates were generated through FEPS. Hourly PM<sub>2.5</sub> emissions are included in Fig. 2. To compare the responsiveness of CMAQ-predicted PM<sub>2.5</sub> concentrations at Atlanta sites to hour-by-hour fire emissions, brute-force sensitivities were estimated for each hour. Perturbations were applied to single-hour emissions in order to quantify first-order sensitivity coefficients and individual hour contributions to PM<sub>2.5</sub> concentrations at downwind receptors. Fig. 12 shows estimated fire contributions to PM<sub>2.5</sub> at South DeKalb for each hour of emissions. At this site most of the fire-related PM<sub>2.5</sub> was attributable to emissions released during a 4-hour span. Emissions released from 12:00 to 16:00 LT accounted for over 85% of the simulated fire contribution to PM<sub>2.5</sub> concentrations.

Differences between fire-related impacts for each hour of emissions are driven by both emissions timing and mass. Sensitivity estimates reflecting concentration responsiveness to fire emissions are more informative. However, an objective comparison between sensitivities to hour-by-hour emission rates must account for the temporal variation in the vertical distribution of emissions as described in Section 3.4.
Once again, a constant vertical distribution was applied to fire emissions to remove the influence of time-varying plume rise profiles and allow sensitivity calculations to focus solely on the temporal allocation of emissions. Fig. 13 shows \( \text{PM}_{2.5} \) concentration sensitivities to hour-by-hour fire emissions at South DeKalb after equally distributing emissions into the 10 lowest vertical layers during the entire simulation. The results at all downwind sites indicate that the sensitivities of modeled \( \text{PM}_{2.5} \) concentrations to hour-specific emissions can differ significantly. In Atlanta, predicted \( \text{PM}_{2.5} \) concentrations were influenced by emissions released between 10:00 and 18:00 LT with concentrations at specific sites responding more intensely to emissions from distinct hours. The analysis also shows that each hour’s fire-related emissions only influenced concentrations at downwind receptors during a 2–3 hour lapse starting approximately 3 h after release. Overall, the sensitivity estimates indicate that the temporal allocation of fire emissions can significantly influence simulated fire-related impacts and peak concentrations. This is in line with findings of the following prior studies. The sensitivity analyses reported by Hodzic et al. (2007) exploring diurnal variability in wildfire emissions showed that hourly resolved smoke emissions can greatly enhance simulations compared to daily inventories. Additionally, improved model predictions have been previously attained by using satellite information to temporally refine fire emissions (Roy et al. 2007). Hu et al. (2008) found from their “hindcast” simulations of this episode that superior model performance may be more readily achieved by improving hourly emission profiles rather than refining fire location or emitted mass.

4. Conclusions

The sensitivity analyses completed in this study demonstrate that successfully modeling the impacts of fires on air quality with regional-scale CTMs depends on effectively allocating the fire emissions in space and time. Furthermore, the results indicate that shortcomings observed in reported simulations cannot be overcome by solely focusing on the magnitude of fire emissions. The horizontal and vertical distributions of emissions on gridded domains and their timing are key inputs that must also be considered.

Here, analyses exploring the influence of plume rise show that modeled \( \text{PM}_{2.5} \) concentrations were mostly sensitive to the fraction of emissions injected into the PBL. The vertical distribution of emissions within the PBL had little effect on downwind concentrations, at least under unstable atmospheric conditions. In the simulations completed, CMAQ-modeled vertical mixing of fire emissions within the PBL was extremely rapid. While correctly determining plume penetration into the free atmosphere is critical, only marginal gains in performance should be expected from applying more detailed representations of vertical plume rise.

Sensitivity estimates related to the horizontal allocation of emissions on a gridded domain indicate that model performance could benefit from more accurately positioning emissions. Predicted \( \text{PM}_{2.5} \) concentrations were sensitive to the horizontal allocation of emissions and responsive to whether fire emissions were horizontally distributed into single or multiple cells. Improving the horizontal allocation of fire emissions may be especially important in relation to plume rise. Using downwind plume rise approximations to vertically distribute fire emissions at the initial position of release is a simplification that may affect model predictions. The responsiveness of simulated \( \text{PM}_{2.5} \) concentrations to small variations in the horizontal allocation of fire emissions also reflects a strong influence from meteorological inputs. Sensitivities may be primarily driven by variability in meteorological fields. Yang et al. (2011) found that errors in CMAQ predictions of the air quality impacts of wildfires may be dominated by uncertainty in wind fields. The degree to which simulations are constrained by uncertainties in meteorological fields produced by weather forecasting models was further investigated in a complimentary paper (Garcia-Menendez et al., 2013). The sensitivity analyses described therein revealed that the inconsistencies between modeled and observed concentrations in the simulated episode were likely driven by uncertainty in meteorological inputs. Nevertheless, uncertainty in the spatiotemporal allocation of fire emissions on modeling domains may exert a significant influence on predicted concentrations comparable to that of uncertainty in the magnitude of emissions.

Perhaps the largest potential gains related to allocation of fire-related emissions lie in better characterizing their temporal distribution. In the simulated episode, sensitivity analyses show that fire-related \( \text{PM}_{2.5} \) impacts were primarily attributable to emissions released within a specific time frame. The analyses also demonstrate that the fire emissions allocated to each hour produced a response at downwind receptors lasting 2–3 h. Reducing the uncertainties associated with distributing emissions into discontinuous inputs and better approximating the
Appendix A. Supplementary data

Supplementary data to this article can be found online at http://dx.doi.org/10.1016/j.scitotenv.2014.05.108.

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