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Linkage between an advanced air quality model and a mechanistic watershed model

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Abstract

An offline linkage between two advanced multi-pollutant air quality and watershed models is presented. The models linked are (1) the Advanced Modeling System for Transport, Emissions, Reactions and Deposition of Atmospheric Matter (AMSTERDAM) (a three-dimensional Eulerian plume-in-grid model derived from the Community Multiscale Air Quality (CMAQ) model) and (2) the Watershed Analysis Risk Management Framework (WARMF). The pollutants linked include gaseous and particulate nitrogen, sulfur and mercury compounds. The linkage may also be used to obtain meteorological fields such as precipitation and air temperature required by WARMF from the outputs of the meteorology chemistry interface processor (MCIP) that processes meteorology simulated by the fifth generation Mesoscale Model (MM5) or the Weather Research and Forecast (WRF) model for input to AMSTERDAM. The linkage is tested in the Catawba River basin of North and South Carolina for ammonium, nitrate and sulfate. Modeled air quality and meteorological fields transferred by the linkage can supplement the conventional measurements used to drive WARMF and may be used to help predict the impact of changes in atmospheric emissions on water quality.

1 Introduction

Watershed models track the fate of water and pollutants in watersheds and associated ecosystems. The proper characterization of dry and wet deposition fluxes of pollutants in such models is important because direct loadings from the atmosphere can have a large contribution to total pollutant loadings, especially in the eastern United States (US). Atmospheric deposition of nitrogen (N) is estimated to contribute 10% to over 40% of new N loadings to estuaries along the eastern US coast and the eastern Gulf of Mexico (Paerl et al., 2002) with contributions of ~38% in the Albemarle-Pamlico Sound in North Carolina and the New York Bight (US EPA, 2008) and as high as ~72% for the St. Catherine-Sapelo estuary in Georgia (Castro et al., 2003). The concentrations of

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sulfate (SO_4^{2-}) in surface waters in the northeastern US have decreased by a third or more in response to decreased emissions and deposition of sulfur (S) from the early 1980s to the mid-1990s (Dennis et al., 2007; US EPA, 2008). Similarly, the contribution of atmospheric mercury (Hg) deposition to elevated aquatic Hg levels is well-known (e.g., Fitzgerald et al., 1998; Lindberg et al., 2007). Hg and S also have a strong relationship in the atmosphere and in the watershed. Atmospheric Hg is converted from the reactive divalent form to elemental form slowly by sulfite ions (van Loon et al., 2000, 2001) and possibly much faster by sulfur dioxide (SO_2) (Seigneur et al., 2006). Also, decreases in S deposition may result in less wetland methylmercury production (Jeremiason et al., 2006).

The calculations of the impacts of sources not discharging directly to the watershed in watershed models are often driven by measurements of pollutant concentrations in air and rain (or of deposition fluxes), and of precipitation and other meteorological fields such as near-ground temperature and wind speed. However, the sparse nature of such measurements could cause error in simulated river flow and pollutant concentrations. Modeled outputs from atmospheric chemical transport models (CTMs) and meteorological models can supplement the observational data input to watershed models. Eulerian CTMs simulate the fate of emissions of atmospheric pollutants in a three-dimensional (3-D) grid by simulating their transport, transformations and deposition to the earth's surface. Such models typically offer greater spatial and temporal resolution than observations. Air quality models (i.e., CTMs) can also be used to simulate the impact of emission controls and long-range transport of pollutants on loadings to watersheds. They also have potential for application in designing emission reduction programs to meet target loads of S and N deposition in a region or ecosystem (Burns et al., 2008).

Several interfaces between air and watershed models have been discussed in the literature. As part of the Chesapeake Bay watershed modeling Program (http://www.chesapeakebay.net/modeling.aspx), a linkage was forged between the Phase 4.2 version of the Chesapeake watershed model and the Regional Acid Deposition

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Model (RADM) (Chang et al., 1987) using geographic information system (GIS) software (Hopkins et al., 2000). The watershed model segments were overlain with the RADM $20 \times 20\,km^2$ grid to determine the percentage of each RADM grid cell falling within each watershed model segment. A similar link was later established (US EPA, 2010) between the Phase 5 Chesapeake Watershed Model and a regression model of monitored wet deposition data refined by deposition fluxes from the US Environmental Protection Agency (EPA) Community Multiscale Air Quality (CMAQ) (Byun and Schere, 2006) model. Burian and co-workers (2004) used an integrated modeling framework composed of the California Institute of Technology (CIT) air quality model, an urban runoff model, and a water-quality model to evaluate the potential impacts of reductions in air emissions of nitrogen oxides (NO_x) and ammonia (NH_3) on the urbanized Los Angeles watershed.

Schwede and co-workers (2009) developed the Watershed Deposition Tool (WDT) which reads processed gridded output of atmospheric deposition from CMAQ and calculates average per unit area and total deposition to selected watersheds and watershed segments based on the area of overlay between each CMAQ grid cell and the polygon for a watershed segment. Sullivan and co-workers (2007, 2008) linked dry and wet S and N deposition fluxes from CMAQ grid cells to equivalent catchments in the biogeochemical model, the Model of Acidification of Groundwater in Catchments (MAGIC) by assuming that the deposition in each grid cell occurred at the center of the cell and developing a raster data set using ArcMap GIS software. CMAQ has also been linked (Brandmeyer et al., 2007) with two watershed models, the Pollutant Loading Model (PLOAD) (US EPA, 2001) and Regional Nutrient Management Model (ReNuMa) (Hong and Swaney, 2007). GIS was used to overlay the CMAQ modeling domain onto the Escambia Bay watershed and apportion the wet and dry N deposition fluxes in the CMAQ grid cells to the polygons representing different land use categories in each subwatershed in the watershed. Annual average wet and dry Hg deposition fluxes from the Regional Lagrangian Model of Air Pollution (RELMAP) (Eder et al., 1986) have been linked with the Watershed Characterization System (WCS) (Greenfield et al., 2002) and

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applied to the Ochlockonee watershed in southern Georgia (Ambrose et al., 2005) to determine the relative importance of atmospheric Hg deposition and terrestrial runoff. The integrated biogeochemical model PnET-BGC has been used to evaluate aquatic ecosystem response to historical and likely future changes in wet and dry deposition of S and N (e.g., Chen and Driscoll, 2004).

Seigneur and Dennis (2010) emphasized the importance of a multipollutant approach to air quality and ecosystem management. In this study, we present a linkage for data transfer between two advanced multi-pollutant air quality and watershed models that facilitates such an approach: (1) The Advanced Modeling System for Transport, Emissions, Reactions and Deposition of Atmospheric Matter (AMSTERDAM) and (2) The Watershed Analysis Risk Management Framework (WARMF).

AMSTERDAM is a state-of-the-science 3-D Eulerian air quality model used to simulate ozone (O_3), particulate matter (PM), and the atmospheric deposition of Hg and acidic and nitrogenous compounds. It is derived from CMAQ and includes an alternative sectional treatment of aerosol processes using the Model of Aerosol Dynamics, Reaction, Ionization and Dissolution (MADRID) (Zhang et al., 2004) and an option for the advanced plume-in-grid treatment (APT) of selected point sources (Karamchandani et al., 2002, 2006). Thus, AMSTERDAM is also referred to as CMAQ-MADRID-APT. Other than differences in aerosol and plume processes, the processes in AMSTERDAM that govern pollutants largely follow those in CMAQ. Like CMAQ, AMSTERDAM treats all major gas-phase air pollutants, including NO_x, SO_2, volatile organic compounds (VOC), carbon monoxide (CO), NH_3 and Hg, as well as O_3, PM and atmospheric deposition, and hence is considered an "one-atmosphere" model because it can simulate the major forms of urban and regional air pollution. AMSTERDAM does not account for the bi-directional exchange of NH_3; Hg re-emission is accounted for explicitly. Different versions of AMSTERDAM have been evaluated against observations of ambient air concentrations of O_3 and fine PM ($PM_{2.5}$) sulfate, nitrate, ammonium, elemental carbon, organic carbon and total mass, and observations of atmospheric deposition of S, N and Hg species (e.g., Bailey et al., 2007; Hu et al., 2008;

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Karamchandani et al., 2002, 2006; Pun et al., 2006; Vijayaraghavan et al., 2006, 2007, 2008; Zhang et al., 2004).

WARMF is an advanced model and decision support system for watershed planning and Total Maximum Daily Load (TMDL) analysis with the capabilities of GIS, graphical user interface (GUI), multiple river basins, and multiple stratified lakes linked by rivers (Chen et al., 2001, 2004a, b, 2008; Herr et al., 2003). WARMF provides a platform to track pollutants, which move with water in time and space over the interconnected terrestrial and aquatic ecosystems. Simulated water quality parameters include major cations, anions, nutrients, dissolved oxygen, organic carbon, suspended sediment, and phytoplankton. Heavy metals and mercury can also be simulated. The model maintains water, heat, and mass balances from atmosphere through canopy, land surface, soil layers, rivers, and lakes. The hydrologic module simulates the processes of canopy interception, snow pack accumulation and snow melt, infiltration through soil layers, evapotranspiration from soil, ex-filtration of ground water to stream segments, kinematic wave routing of stream flows, and flow routing of the terminal reservoir (Chen et al., 2001). Along each flow path, the chemistry module in WARMF performs mass balance and chemical equilibrium calculations to account for the processes of dry deposition to the canopy, nitrification of ammonia on the canopy, ion leaching from sap to the canopy surface, wash-off by throughfall, ion leaching by snowmelt, and the soil processes, e.g. litter fall, litter breakdown, litter decay, nitrification, denitrification, cation exchange, anion adsorption, weathering, and nutrient uptake. More detailed information on the governing equations in WARMF can be found elsewhere (Chen et al., 2001).

Meteorology needed by AMSTERDAM is obtained from the Fifth Generation Penn State University/National Center for Atmospheric Research Mesoscale Model (MM5) (Grell et al., 1995) or the Weather Research and Forecast (WRF) Model's Advanced Research WRF (ARW) core (Skamarock et al., 2008) and processed using the Meteorology Chemistry Interface Processor (MCIP) (Otte and Pleim, 2009) to create air quality model-ready gridded fields. WARMF is driven by time series data for meteorology, precipitation chemistry and air quality. Meteorology data are traditionally obtained

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from the National Climatic Data Center (NCDC) Summary of the Day dataset (NCDC, 2009) and precipitation chemistry and air quality data are obtained from the National Atmospheric Deposition Program (NADP) monitoring stations (http://nadp.sws.uiuc.edu) and the Clean Air Status and Trends Network (CASTNET) (www.epa.gov/castnet), respectively. Here, we take advantage of the fact that some of the data needed to drive WARMF are also available from the output of air quality and meteorological models such as AMSTERDAM and MM5/WRF/MCIP, respectively.

We describe below the development and testing of a linkage for offline data transfer from AMSTERDAM and MCIP output to WARMF. The linkage connects the mechanistic multi-pollutant WARMF model with an air quality model for the first time and has several additional special features, one or more of which are absent in the other linkages reported above. These features include: (1) the ability to read air quality output files in their native format (here, I/OAPI netCDF – Input Output Applications Programming Interface Network Common Data Form) instead of requiring prior conversion of air quality model outputs to ASCII text or spreadsheet-based formats, (2) consistency between the meteorology used to drive the air quality and watershed models, (3) the inclusion of gaseous and particulate S, Hg, and oxidized and reduced N species, (4) a distinction between fine and coarse PM, and (5) applicability to any watershed (with available calibrated WARMF data and a spatially overlapping AMSTERDAM modeling domain).

We first describe the procedure for mapping the data between the different models and the issues that need to be considered in such an exercise and then provide an example application of the linkage.

2 Description of linkage

The AMSTERDAM-WARMF linkage processes the atmospheric concentrations and wet and dry deposition fluxes simulated by AMSTERDAM and the meteorological fields output by MCIP and creates the input files required by WARMF. The coupling

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is one-way, i.e., information is transferred from AMSTERDAM and MCIP to WARMF. Figure 1 presents an overview of the different components of the linkage. WARMF requires three groups of input files for atmospheric deposition impact calculations: (1) ".air" files which contain atmospheric concentrations and concentrations in precipitation of gases and fine PM, and *.cpa files which similarly contain atmospheric and concentrations in precipitation of coarse PM, (2) ".ddepv" files which provide dry deposition velocities and (3) ".met" files which contain meteorological data (Chen et al., 2001). The linkage consists of FORTRAN code and UNIX shell scripts that create these three groups of input files after reconciling differences between AMSTERDAM/MCIP and WARMF in spatial and temporal resolution and extent and the representation of meteorological variables and chemical species, as described below.

2.1 Spatial resolution and extent

WARMF is a GIS-based watershed model, i.e., the compartments of a river basin are spatially referenced by their coordinates and linked. The model is not based on a uniform grid but rather on a network of continuously stirred tank reactors (CSTRs) comprising compartments that include irregularly spaced land catchments, river segments and lake segments, usually 1 km^2 or larger. The network of CSTRs allow water and associated pollutants to be transported from one to another. In contrast, the AMSTERDAM and MCIP outputs are available in rectangular grid cells usually projected in a lambert conformal projection system. The horizontal grid resolution is typically $4 \times 4\,km^2$, $8 \times 8\,km^2$, $12 \times 12\,km^2$ or $36 \times 36\,km^2$. There are several vertical levels with varying thicknesses that extend up to the tropopause. The surface layer, which interacts with water bodies, is typically 30 to 40 m thick.

Selected variables (described below) in the surface layer of AMSTERDAM/MCIP output files are mapped to the WARMF modeling domain in the following manner. AMSTERDAM grid cells that lie in the rectangular sub-domain enclosing the WARMF watershed are first identified to allow the processing of AMSTERDAM results over a smaller sub-domain that encompasses the watershed rather than the entire domain.

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In the default application of WARMF, each catchment and reservoir is assigned to the nearest rain/air quality station and the nearest meteorology station. Meteorology data are also adjusted for each catchment and reservoir by a precipitation multiplier and a temperature lapse to account for differences between the assigned meteorology station and the climatic characteristics of the catchment. The catchment's average precipitation is determined using the inverse distance weighted average of all stations in the vicinity. The precipitation multiplier is applied to the assigned meteorology station's data in order to maintain that catchment's average characteristics. The temperature lapse is calculated based on catchment elevation and a constant altitudinal temperature gradation. To exploit this formulation in WARMF, the linkage code creates "pseudo-stations", one for each grid cell in the AMSTERDAM sub-domain, with latitude/longitude corresponding to the grid cell center. Meteorological and air quality model output are provided at each pseudo-station to WARMF for subsequent processing. Meteorology and air concentrations are extracted only from the first vertical level of AMSTERDAM output, so no vertical mapping is needed.

2.2 Temporal resolution and extent

WARMF timescales range from hourly to multi-year as ecosystems typically react over long time scales (from several years to over a hundred years) while the output resolution of AMSTERDAM and MCIP is hourly because the impacts of the emissions, transport and transformations of pollutants are often seen quickly in the atmosphere. AMSTERDAM simulations can be conducted for any time period; however, outputs from annual or multi-year simulations are more appropriate for input to WARMF due to the long timescales typically used in ecosystem modeling. Multi-year air quality model simulations are uncommon as they are limited by the availability of historical year-specific emissions data but they could be useful in modeling the impact of projected long-term emissions or climate change on hydrology and chemistry. While the internal processes in AMSTERDAM and WARMF occur at various time steps as discussed above, the transfer of information in the linkage is performed at a 1-h resolution. The linkage

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software provides hourly outputs from AMSTERDAM and MCIP to WARMF which then performs necessary temporal aggregation. The time zone of the WARMF application is specified by the user. MCIP and AMSTERDAM outputs are in Greenwich Mean Time (GMT) and are converted to local standard time as required by WARMF.

2.3 Meteorology

Meteorological fields required by WARMF include precipitation, temperature, cloud cover, dew point temperature, air pressure, and wind speed. WARMF accepts daily or hourly meteorological data as input and calculates canopy interception, snowmelt, evapotranspiration, soil moisture, ground-water percolation, lateral ground-water flow, ground-water table elevation, surface runoff, stream flow and lake hydrodynamics. Precipitation amounts and dry deposition velocities are combined with other inputs of atmospheric gaseous, particulate, and precipitation concentrations of chemical species to determine the loading entering the watershed in dry and wet deposition.

The hourly meteorological fields required by WARMF are processed from the MCIP output files taking into account the differences in spatial and temporal resolution and extent as described above. Table 1 shows the MCIP meteorological fields used to develop the necessary WARMF fields. Here, METCRO2D and METCRO3D refer to the temporally varying 2-D and 3-D gridded MCIP meteorological outputs. The MCIP and AMSTERDAM output files are available in I/OAPI netCDF format. The linkage converts data are converted from this format to the ASCII format of the WARMF input files. Hourly precipitation is calculated from the sum of convective and non-convective precipitation fields (RC and RN, respectively) available from MCIP. WARMF requires daily minimum and maximum temperatures or, equivalently, temperatures at every hour which can then be processed to determine the daily range. Hourly temperatures are obtained from the MCIP field TEMP2, the air temperature at 2 m height above ground. The 2 m height corresponds approximately to the height at which ambient temperature sensors are located. Thus, the modeled variable TEMP2 is analogous to the temperature observations normally input to WARMF. The cloud cover fraction is directly available from

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MCIP. Dew point temperature (T_d) is calculated from the surface pressure (PRSFC) and water vapor mixing ratio (QV) from the METCRO2D file and the surface layer of the METCRO3D file, respectively, using the following analytical approximation (Rogers and Yau, 1989):

$$T_d = B/\ln(A^*0.622/w^*p) \quad (1)$$

where B = 5420 K; $A = 2.53 \times 10^8$ kPa; w = water vapor mixing ratio (in kg/kg); p = local pressure (in kPa).

The last two meteorological fields listed in Table 1, pressure and wind speed are extracted directly from the variables PRSFC and WSPD10 (wind speed at 10 m height above ground) in the METCRO2D file.

Errors in the MM5/WRF-MCIP prediction of precipitation will propagate into error of simulated flow in the watershed model (e.g., Herr et al., 2010). This is particularly important when large discrepancies are noted between the modeled precipitation rates and rain gage measurements. In general, there is a trade-off between greater spatial coverage available from modeled meteorology and potential errors in precipitation predictions. Golden and co-workers (2010) used stream gage measurements in two watersheds in N. Carolina to evaluate runoff in a grid-based watershed mercury model (GBMM) with precipitation from (1) MM5, (2) the Parameter-elevations Regressions on Independent Slopes Model (PRISM) (Daly et al., 2002), and (3) weather radar-based multi-sensor National Precipitation Analysis Stage IV (NPA) data (http://www.emc.ncep.noaa.gov/mmb/research/stage4.FAQ.html). Based on their results, they suggest that linking CMAQ outputs with watershed models is reasonable for assessment studies but that MM5 precipitation and CMAQ deposition data should not be used for calibrating the watershed model.

2.4 Chemical species

WARMF can use hourly atmospheric concentrations of the following species in the *.air file for each pseudo-station: NH_3, NO_x, nitric acid (HNO_3), other NO_z (i.e., sum

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of all oxidized N species other than NO_x and HNO_3), SO_2, elemental mercury (Hg^0), gaseous divalent mercury (Hg^{II}), and the following $PM_{2.5}$ components: ammonium (NH_4^+), nitrate (NO_3^-), sulfate (SO_4^{2-}), sodium (Na^+), potassium (K^+), calcium (Ca^{2+}), magnesium (Mg^{2+}), and chloride (Cl^-). WARMF also requires concentrations in precipitation of total ammonium (NH4), NO_x, total nitrate (NO_3), other NO_z, SO_2, total sulfate (SO4), HG^{II}, and the $PM_{2.5}$ components listed above. WARMF also uses air and precipitation concentrations of coarse PM ($PM_{10-2.5}$) $SO_4^=$, NO_3^- and NH_4^+. WARMF can also accept daily or irregular (instead of hourly) concentrations but that option is not used when it is linked to the air model.

The mapping of chemical species between the AMSTERDAM output files and WARMF *.air files is shown in Tables 2 and 3 for atmospheric concentrations and precipitation concentrations, respectively. The mapping for coarse PM concentrations is shown in Table 4. All concentrations are expressed in $\mu g/m^3$; gas-phase concentrations are converted from ppmV to $\mu g/m^3$ using the temperature and pressure in the MCIP METCRO2D file. Concentrations in precipitation are calculated from the AMSTERDAM wet deposition fluxes and the MCIP precipitation fields. Air and precipitation concentrations of SOX and SO4 are reported as S, NO_x and HNO3 as NO_2, NH3 as NH_3, and other N species as N. All of the species required by WARMF are available in AMSTERDAM except K^+, Ca^{2+}, and Mg^{2+}. Na^+ and Cl^- are simulated by AMSTERDAM; however, due to uncertainty in the emissions inventory used to drive Na^+ and Cl^- concentrations in AMSTERDAM, WARMF continues to use CASTNET observational data for these species as it does for K^+, Ca^{2+}, and Mg^{2+}. Because WARMF can read both observations and model outputs processed by the linkage for the same species if necessary, there is the potential for data fusion to leverage the positive attributes of both modeled and measured data.

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2.5 Dry deposition velocities

The deposition velocity module of the linkage creates files with monthly average dry deposition velocities of gases and fine and coarse PM that are input to WARMF. The dry deposition velocities and air concentrations are used in WARMF to calculate dry deposition. Table 5 shows the dry deposition velocity species mapping between AMSTERDAM and WARMF species. A single monthly value is specified for the dry deposition velocity of each species in the linkage and is calculated from the average of the monthly averages across all grid cells in the watershed. The dry deposition velocities of the nitrogen groups, OTHNOZ and NOX, are calculated from the total AMSTERDAM dry deposition flux summed across the relevant individual species and the atmospheric mass concentration summed across these species simulated in the surface layer. The dry deposition velocities of the gases input to WARMF other than NOX and OTHNOZ are calculated from the hourly dry deposition velocity in the METCRO2D file. Future versions of MCIP may not provide the dry deposition velocities of gases; these may instead be calculated only within the air quality model (Otte and Pleim, 2010). In this case, the linkage code will need to be modified to calculate dry deposition velocities of all gases from the corresponding dry deposition flux and mass concentration as is done now for OTHNOZ and NOX. Also, because Hg^0 dry deposition velocities in MCIP versions 3.0 and earlier are not correct (R. Bullock, EPA, personal communication, 2009), the linkage includes a provision for using a constant Hg^0 dry deposition velocity of 0.01 cm/s (Seigneur et al., 2004) for those MCIP versions. The dry deposition velocities of fine and coarse PM, referred to PARTDV and COARSEDV in WARMF, are set equal to the dry deposition velocities of fine and coarse particulate elemental (black) carbon (EC_1 and EC_2) which are, in turn, calculated from the respective dry deposition fluxes and air concentrations.

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3 Testing of the linkage

3.1 Overview

The AMSTERDAM-WARMF linkage is tested in the Catawba River watershed in North and South Carolina for the 2002 calendar year. While multi-year simulations are more appropriate to test watershed responses, our purpose here is only to demonstrate a proof-of-application of the linkage. 2002 was a slightly dry to normal year for the Catawba basin based on the average precipitation from 1950 to 2007 (NOAA, 2008). The Catawba basin and the 2002 period were selected to test the linkage because prior air and water model applications were available for this region and time period. WARMF has been previously applied in the Catawba watershed (Weintraub, 2005). Also, AMSTERDAM and MCIP outputs are available for 2002 over an air quality modeling domain that includes this geographic area (Vijayaraghavan et al., 2010).

Figure 2 shows the air quality and watershed modeling domains used for testing the linkage. The AMSTERDAM domain grid has a horizontal resolution of 12 km and a vertical grid structure consisting of 19 layers from the surface to an altitude of ~14 km with finer resolution near the surface; the surface layer is approximately 35 m thick. The version of AMSTERDAM used here is based on CMAQ v.4.6. Meteorology is driven by MM5 (Olerud and Sims, 2004) and emissions developed by the Visibility Improvement State and Tribal Association of the Southeast (VISTAS) Regional Planning Organization (MACTEC, Inc., 2008). The WARMF domain is in the northeastern part of the AMSTERDAM domain and covers the Catawba River and its watershed. The headwaters of the Catawba River are in the Blue Ridge Mountains to the northwest. The Catawba flows east and then south through the Piedmont region of the Carolinas, past the city of Charlotte, North Carolina. There are 11 dams forming reservoirs on the Catawba River, the last of which is Lake Wateree in South Carolina.

A simulation was conducted in addition to the baseline (WARMF default) scenario to identify the differences in atmospheric deposition, precipitation, hydrology, and water quality when using AMSTERDAM and MCIP meteorology and air/rain chemistry

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compared to the WARMF baseline scenario that is driven by only measurements. Table 6 shows the two scenarios run. The Catawba River WARMF application includes 650 land catchments, 566 river segments, and 11 reservoirs. Four subwatersheds were chosen within this watershed to provide a representative and broad selection of locations. The locations are shown with red dots in Fig. 3 and are described in Table 7. The detailed land use breakdown of each subwatershed is shown in Table 8. The land use patterns range from predominantly forested mountains (Linville River) to rural forested and agricultural (South Fork Catawba River) and from urban (Sugar Creek) to mixed use (Lake Wateree).

To evaluate the effect of the AMSTERDAM-WARMF linkage on watershed simulations, the simulation results were compared against each other and against observed data, where available, for those parameters directly affected by the linkage. Ammonia, nitrate, and sulfate are the primary chemical species directly impacted by the linkage. The linkage for mercury between the models is also available, but the WARMF model has not been calibrated for mercury simulation in the Catawba basin and hence mercury species are not examined below. The impact of using MM5/MCIP portion of the linkage on flow rates in the Catawba River basin is discussed elsewhere (Herr et al., 2010). Below, we present a discussion of the impacts of using the linkage on deposition fluxes and water quality.

3.2 Ammonia

Within WARMF, "ammonia" is expressed as ammonium ion, which is the dominant form at pH levels commonly seen in aquatic environments. Gaseous ammonia is assumed to be converted to ammonium upon contact with canopy, soil, or surface water. Atmospheric sources of ammonia include wet deposition of dissolved ammonium ion in precipitation and dry deposition of fine and coarse particles and ammonia gas.

The results of the simulations are presented from upstream to downstream in the Catawba River watershed in the four panels in Fig. 4. Shown in each panel are the ammonia concentrations in water simulated using (1) observed precipitation

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concentrations from NADP, air concentrations from CASTNET, and meteorology at NCDC monitoring stations (i.e., the WARMF baseline application), and (2) modeled air/rain concentrations, dry deposition velocities, and meteorology from AMSTERDAM and MCIP (i.e., the air model linkage scenario). Also shown are observations for ammonia concentrations from North Carolina Department of Water Quality (NCDENR) and EPA Storage and Retrieval (STORET) database (http://www.epa.gov/storet/), where available. The two model scenarios shown correspond to those listed in Table 6. Table 9 presents the annual average ammonia concentration in the two scenarios in each subwatershed. Table 10 shows the wet and dry deposition fluxes calculated by WARMF in these two scenarios as well as the deposition fluxes output from AMSTERDAM.

As seen in Fig. 4, predicted concentrations at Linville River in the air model linkage scenario are almost always higher than those in the baseline scenario with the annual average concentration more than twice that in the linkage scenario (Table 9). The annual dry deposition calculated in WARMF in the linkage scenario is 30% less than that in the baseline scenario (0.40 vs. 0.62 kg/ha/yr) (Table 10) while the annual wet deposition in WARMF in the linkage scenario is more than twice than the baseline WARMF value, indicating that differences in wet deposition are primarily responsible for the higher water concentrations in the linkage scenario. Wet and dry deposition fluxes output by AMSTERDAM are also shown in Table 10. These are comparable to the fluxes calculated in WARMF in the linkage scenario for this subwatershed.

Predicted ammonia concentrations in the South Fork Catawba River are sometimes higher in the linkage scenario and sometimes in the baseline WARMF application, but the values in both scenarios are typically higher than the observed values with neither scenario consistently out-performing the other (Fig. 4). Notwithstanding the fact that annual wet and dry deposition fluxes calculated in WARMF in the linkage scenario are both more than twice than those in the baseline WARMF case (Table 10), the annual average ammonia concentrations in water are equal in the two scenarios (Table 9). This suggests that atmospheric deposition may not be the primary contributor

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to ammonia loading in this subwatershed. This is also true of Sugar Creek and Lake Wateree where again annual wet and dry deposition fluxes in the linkage scenario are 2 to 8 times those in the baseline case (Table 10), but annual average concentrations are either similar in the two scenarios (Sugar Creek) or lower in the linkage scenario (Lake Wateree) (Table 9). Also, while the annual wet deposition flux output by AMSTERDAM is comparable to that calculated in WARMF in the linkage scenario for these two watersheds, annual dry deposition is approximately half in the AMSTERDAM output than that calculated in WARMF in the linkage scenario (Table 10). This highlights the differences in the treatment of dry deposition in AMSTERDAM and WARMF; for example, though dry deposition velocities that vary with location and hour are available and used by AMSTERDAM in dry deposition flux calculations, WARMF requires monthly average dry deposition velocities that are constant over the entire Catawba watershed and hence an average value over the Catawba watershed is provided by AMSTERDAM to WARMF via the linkage.

3.3 Nitrate

Within WARMF, "nitrate" refers to all dissolved inorganic oxidized nitrogen. Although other forms like nitrite are present in small quantities, aquatic reactions quickly covert these forms to nitrate ion. Gaseous oxidized forms of nitrogen are assumed to be converted to nitrate upon contact with canopy, soil, or surface water. Atmospheric sources of nitrate include wet deposition of dissolved nitrate ion in precipitation, particulate dry deposition with fine and coarse particles, and deposition of NO_x, HNO_3 and other NO_z gases. Nitrate concentrations in water in the four subwatersheds in the WARMF baseline and linkage scenarios and from NCDENR and STORET observations, where available, are shown in Fig. 5. Annual average concentrations in the two scenarios are shown in Table 11. Annual wet and dry deposition fluxes calculated in WARMF in the two scenarios and those output from AMSTERDAM are listed in Table 12.

Linville River has naturally lower nutrient concentrations than South Fork and Sugar Creek and thus the nitrate concentrations simulated in WARMF are more sensitive to

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atmospheric loading as seen in Table 11. Figure 5 shows that concentrations in the Linville River in the linkage scenario are consistently higher (and sometimes greater than 5×) than the baseline. As seen in Table 12, both the WARMF linkage scenario and AMSTERDAM simulate twice as much annual wet deposition as the WARMF baseline. They also simulate two orders of magnitude more dry deposition than the WARMF baseline because the baseline uses a gaseous dry deposition velocity of 0.001 cm/s, which is about 1/100th the deposition velocity provided by AMSTERDAM, and because WARMF accounts for coarse PM nitrate in the linkage scenario. Despite these large differences in deposition between the WARMF baseline and linkage scenarios, annual average concentrations do not change by more than 15% in South Fork, Sugar Creek and Lake Wateree reflecting the smaller role that atmospheric deposition plays in total nitrate loading in these three subwatersheds. Neither the WARMF baseline nor linkage scenario performs consistently better than the other when compared against observations of nitrate concentrations in water.

The annual wet deposition calculated by WARMF in the linkage scenario is lower than but within 10% of that predicted by AMSTERDAM (Table 12). The calculated dry deposition flux of nitrate is within 6% between the two models in the mountain watershed of Linville River but in the remaining watersheds with more varied land use, WARMF calculates 8 to 28% more dry deposition of nitrate in the linkage scenario than AMSTERDAM.

3.4 Sulfate

Sulfate is the only form of inorganic sulfur simulated by WARMF, and it is the form of sulfur which dominates in aquatic environments. SO_2 is assumed to be rapidly converted to sulfate upon contact with canopy, soil, or surface water. Atmospheric sources of sulfate include wet deposition in precipitation, particulate dry deposition with fine and coarse particles, and deposition of SO_2. Time series of sulfate concentrations in water from upstream to downstream in the WARMF baseline and linkage scenarios are shown in Fig. 6. Observations of concentrations are not available. Annual

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average concentrations in the two scenarios are listed in Table 13. Annual wet and dry deposition fluxes calculated in WARMF in the two scenarios and those output from AMSTERDAM are shown in Table 14.

Predicted concentrations in water in Linville River, South Fork and Sugar Creek are not consistently higher in either the WARMF baseline or the linkage scenario as illustrated in Fig. 6. Annual average concentrations in the South Fork Catawba River, Sugar Creek and Lake Wateree are 5% to 33% higher in the linkage scenario than in the baseline (Table 13) reflecting, in part, the higher wet and dry deposition in the linkage scenario (Table 14).

The wet deposition calculated by WARMF in the linkage scenario is less than, but within 10% of, that predicted by AMSTERDAM (Table 14). The dry deposition calculated in WARMF in the linkage scenario is 25% to 45% less than the dry deposition predicted by AMSTERDAM. Both simulations have much higher dry deposition flux than the WARMF baseline simulation because the WARMF baseline uses a very low gas deposition (only 0.001 cm/s) instead of 0.5 cm/s to 0.7 cm/s as used in AMSTERDAM.

4 Summary

The linkage between AMSTERDAM and WARMF enables the transfer of data on simulated atmospheric gaseous, particulate, and precipitation concentrations that drive wet and dry deposition fluxes from the air to the watershed model after reconciling differences in spatial and temporal resolution and chemical species representations between the two models. The linkage and the two models linked thus allow us to follow the path of pollutants emitted into the air, their transport and transformations in the atmosphere, their deposition to the Earth and fate in water bodies/watersheds after interactions with other anthropogenic and biogenic matter. The linkage may also be used to transfer modeled meteorological fields from MCIP (originally derived from either MM5 or WRF) to WARMF. Employing the same meteorology in the air and watershed models

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helps avoid the inconsistency that would otherwise result in addressing the effects of change in deposition loading between current conditions based on measurements and future conditions based on meteorological/air quality modeling. The meteorology linked includes near-ground temperature, precipitation, cloud cover fraction, dew point temperature, pressure and wind speed.

The AMSTERDAM-WARMF linkage also can be used to connect individual atmospheric point sources to water quality consequences. This is important because regulation of water quality is based on individual impaired river reaches and lakes. In cases where the water quality impairment is due at least in part to atmospheric deposition, a linkage needs to be established to determine the effect of atmospheric emitters on water quality. The spatially detailed AMSTERDAM air quality model uses emissions from point and other sources as well as meteorology as model inputs and produces atmospheric concentrations and deposition to the land surface as output. WARMF takes gaseous air quality, particulate air quality, rain quality, and local meteorology as input and generates water quality as output. Linking the two types of models together provides a rigorous scientific framework to quantify an emitter's effects on air and water and support pollution trading between atmospheric and watershed point sources. Such information is also useful for source attribution analyses in current year and future emission control scenarios.

Testing of the linkage in the Catawba River watershed showed that large differences could sometimes exist in water quality concentrations simulated by WARMF when using AMSTERDAM/MCIP outputs instead of the default monitoring data. These differences could be attributed to differences in the input data and model treatments. Caution is advised when using modeled air quality and meteorological fields in watershed modeling as these are estimates derived from numerical representations of atmospheric physics and chemistry. Nonetheless, they offer the advantage of significantly greater spatial coverage and resolution than field measurements and are particularly useful in estimating the effect of atmospheric emissions on water quality after the proposed implementation of controls or due to climate change. Hence, modeled

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atmospheric and meteorological fields transferred by the linkage are recommended as a supplement to conventional measurements used to drive WARMF and other watershed models.

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Table 1. Mapping between WARMF and MCIP meteorological fields in the WARMF *.met file.

WARMF field	Units	MCIP field(s)	MCIP/AMSTERDAM file name(s)
Precipitation	cm/hr	Convective + Non-convective precipitation (RC + RN)	METCRO2D
Temperature	˚C	Air temperature at 2 m elevation (TEMP2)	METCRO2D
Cloud cover fraction		Total cloud fraction (CFRAC)	METCRO2D
Dew point T (T_d)	˚C	Surface pressure (PRSFC) and Water vapor mixing ratio (QV) $T_d = f$(PRSFC, QV)	METCRO2D (PRSFC) METCRO3D (QV)
Pressure	mb	Surface pressure (PRSFC)	METCRO2D
Wind speed	m/s	Wind speed at 10 m (WSPD10)	METCRO2D

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Table 2. Mapping between WARMF and AMSTERDAM chemical species names for atmospheric concentrations of gases and fine particles ($PM_{2.5}$) in the WARMF *.air file.

WARMF Species Name	AMSTERDAM Species Name
Gases	
NH3	NH3
NOX	NO + NO2
HNO3	HNO3
OTHNOZ [a]	HONO + NO3 + 2 x N2O5 + PNA + PAN + NTR
SOX	SO2
HG0	HG0
HGII	HG2
$PM_{2.5}$	
NH4	NH4_1
NO3	NO3_1
SO4	SO4_1
NA, K, CA, MG, CL	N/A (use CASTNET data in WARMF)

[a] OTHNOZ is an abbreviated form of "other NOz"

HG0 = elemental mercury; HG2 = HGII = Divalent mercury; HONO = nitrous acid; HNO3 = Nitric acid; N2O5 = dinitrogen pentoxide; NH3 = Ammonia; NH4 = NH4_1 = $PM_{2.5}$ ammonium; NO = Nitric oxide; NO2 = Nitrogen dioxide; NO3 (gas) = nitrogen trioxide; NO3 ($PM_{2.5}$) = NO3_1 = $PM_{2.5}$ nitrate; NOX = Nitrogen oxides; NTR = alkyl nitrate; PAN = peroxyacyl nitrates; PNA = peroxy nitric acid; SO2 = SOX = sulfur dioxide; SO4 = SO4_1 = $PM_{2.5}$ sulfate.

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Table 3. Mapping between WARMF and AMSTERDAM chemical species names for precipitation concentrations in the WARMF *.air file.

WARMF Species Name	AMSTERDAM Species Name
NH4	NH3 + NH4_1 + NH4_2
NOX	NO + NO2
NO3	HNO3 + NO3_1 + NO3_2
OTHNOZ [a]	HONO + NO3 + 2 x N2O5 + PNA + PAN + NTR
SOX	SO2
SO4	SO4_1 + SO4_2
HGII	HG2 + HGP_1 + HGP_2
NA, K, CA, MG, CL	N/A (use NADP data in WARMF)

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Table 4. Mapping between AMSTERDAM and WARMF chemical species names for atmospheric concentrations and precipitation concentrations of coarse particles ($PM_{10-2.5}$) in the WARMF *.cpa file.

WARMF Species Name	AMSTERDAM Species Name
NH4	NH4_2
NO3	NO3_2
SO4	SO4_2

NH4 = NH4_2 = $PM_{10-2.5}$ ammonium; NO3 = NO3_2 = $PM_{10-2.5}$ nitrate; SO4 = SO4_2 = $PM_{10-2.5}$ sulfate.

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Table 5. Mapping between AMSTERDAM and WARMF chemical species names for dry deposition velocities in the WARMF *.ddepv file.

WARMF Species Name	AMSTERDAM Species Name
SOX	SO2
NOX	NO, NO2
HNO3	HNO3
OTHNOZ	NO3, N2O5, HONO, PAN, NTR
NH3	NH3
HG0	HG0
HG2	HG2
PARTDV	EC_1
COARSEDV	EC_2

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Table 6. WARMF simulations.

Case	Air/Rain Chemistry, Atmospheric Deposition	Meteorology
Baseline (WARMF default)	CASTNET, NADP	NCDC
Air model linkage scenario	AMSTERDAM	MCIP

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Table 7. Descriptions of Catawba River testing location subwatersheds.

Location	Watershed Description
Linville River	Mountain river
South Fork Catawba River	Rural forest & agriculture
Sugar Creek	Urban (city of Charlotte)
Lake Wateree	Mixed

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Table 8. Land uses of the testing location subwatersheds.

Land Use	Linville River	South Fork Catawba R.	Sugar Creek	Lake Wateree
Deciduous Forest	41.6%	25.8%	14.8%	30.4%
Evergreen Forest	21.1%	18.8%	7.5%	22.9%
Mixed Forest	29.1%	14.3%	2.6%	11.8%
Grassland	0.0%	0.0%	1.2%	2.1%
Shrub/Scrub	0.0%	0.0%	0.2%	0.3%
Wetlands	0.2%	0.5%	0.7%	0.8%
Herbaceous Wetland	0.0%	0.0%	0.0%	0.0%
Pasture	2.7%	16.4%	4.6%	12.0%
Cultivated	1.6%	14.0%	1.1%	5.2%
Recreational Grasses	1.0%	0.8%	26.3%	4.7%
Low Intensity Developed	1.6%	5.1%	23.3%	5.2%
Med. Intensity Developed	0.0%	0.0%	6.7%	0.8%
High Intensity Developed	0.0%	0.9%	6.9%	1.0%
Commercial / Industrial	0.7%	2.6%	3.4%	1.4%
Barren	0.5%	0.4%	0.4%	0.5%
Water	0.2%	0.3%	0.3%	0.9%

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Table 9. Annual average ammonia concentration (mg/L N) in baseline WARMF simulation and air model linkage scenario.

Subwatershed	Baseline (WARMF default)	Air model linkage scenario
Linville River	0.13	0.27
S. Fork Catawba R.	0.33	0.33
Sugar Creek	0.83	0.82
Lake Wateree	0.13	0.10

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Table 10. Annual wet and dry deposition flux of ammonia (kg/ha/year as N).

Subwatershed	Input to WARMF (Baseline WARMF default)	Input to WARMF (Air model linkage scenario)	AMSTERDAM output
Wet Deposition			
Linville River	0.74	1.66	1.68
S. Fork Catawba R.	0.83	1.71	1.78
Sugar Creek	0.80	2.14	2.22
Lake Wateree	0.79	1.82	1.90
Dry deposition			
Linville River	0.62	0.40	0.34
S. Fork Catawba R.	0.54	1.40	0.90
Sugar Creek	0.36	2.95	1.47
Lake Wateree	0.55	2.24	1.14

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Table 11. Annual average nitrate concentration (mg/L N) in baseline simulation and air model linkage scenario.

Subwatershed	Baseline (WARMF default)	Air model linkage scenario
Linville River	0.45	1.17
S. Fork Catawba R.	1.28	1.42
Sugar Creek	5.66	5.50
Lake Wateree	0.43	0.42

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Table 12. Annual wet and dry deposition flux of nitrate (kg/ha/year as N).

Subwatershed	Calculated by WARMF (Baseline WARMF default)	Calculated by WARMF (Air model linkage scenario)	AMSTERDAM output
Wet Deposition			
Linville River	1.02	1.93	2.10
S. Fork Catawba R.	1.18	2.17	2.30
Sugar Creek	1.10	2.14	2.28
Lake Wateree	1.09	2.03	2.17
Dry deposition			
Linville River	0.05	5.09	5.38
S. Fork Catawba R.	0.04	6.99	5.47
Sugar Creek	0.03	8.62	7.77
Lake Wateree	0.04	6.34	5.87

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Table 13. Annual average sulfate concentration (mg/L S) in baseline simulation and air model linkage scenario.

Subwatershed	Baseline (WARMF default)	Air model linkage scenario
Linville River	4.77	4.36
S. Fork Catawba R.	3.10	3.71
Sugar Creek	0.77	0.81
Lake Wateree	0.96	1.28

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Table 14. Annual wet and dry deposition flux of sulfate (kg/ha/year as S).

Subwatershed	Input to WARMF (Baseline WARMF) default	Input to WARMF (Air model linkage) scenario	AMSTERDAM output
Wet Deposition			
Linville River	2.29	5.32	5.37
S. Fork Catawba R.	2.69	4.89	5.31
Sugar Creek	2.49	5.57	6.16
Lake Wateree	2.48	4.86	5.35
Dry deposition			
Linville River	0.19	2.40	4.40
S. Fork Catawba R.	0.17	3.43	4.56
Sugar Creek	0.11	5.58	8.77
Lake Wateree	0.17	3.59	5.44

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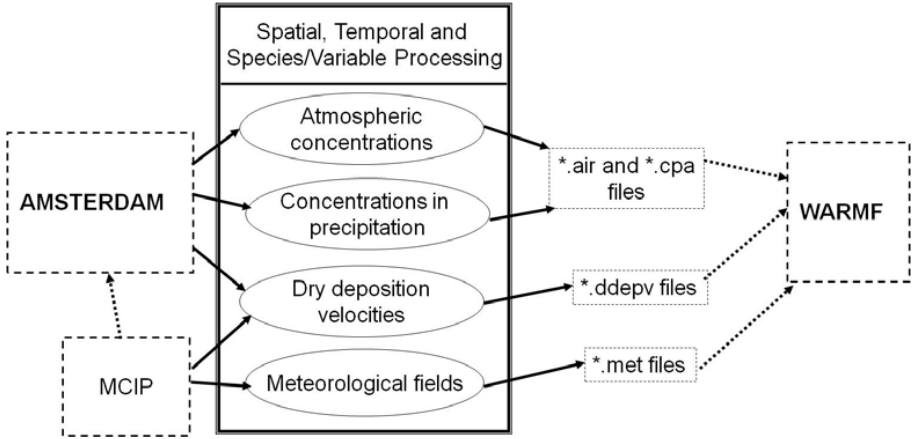

Fig. 1. Overview of the AMSTERDAM-WARMF linkage.

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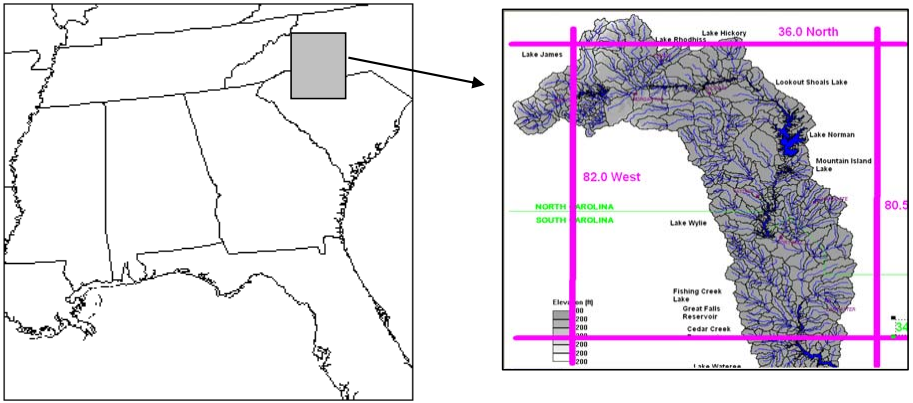

Fig. 2. Air quality domain (left) and Catawba River watershed modeling domain (right).

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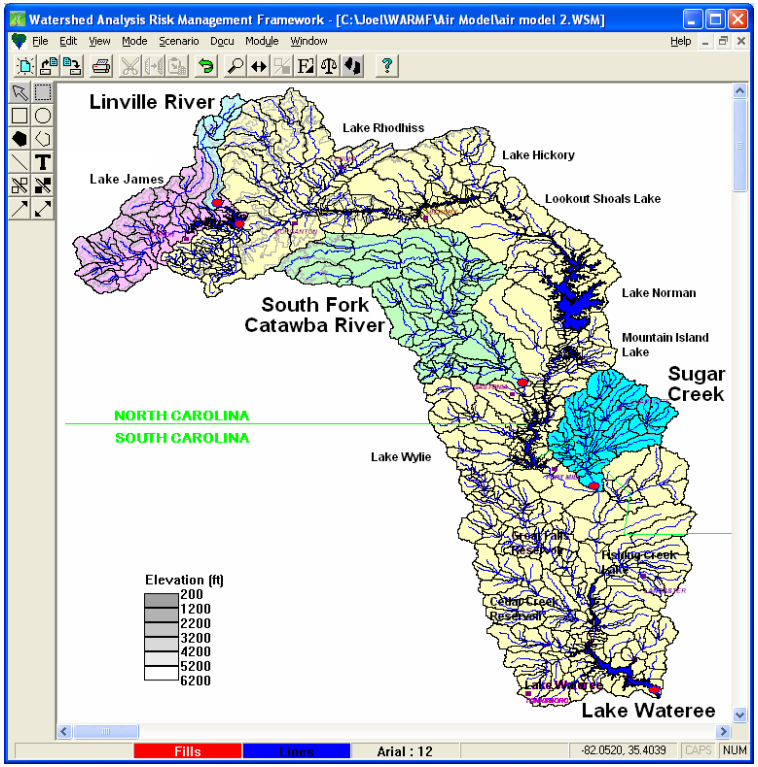

Fig. 3. WARMF screen snapshot showing testing locations and subwatersheds.

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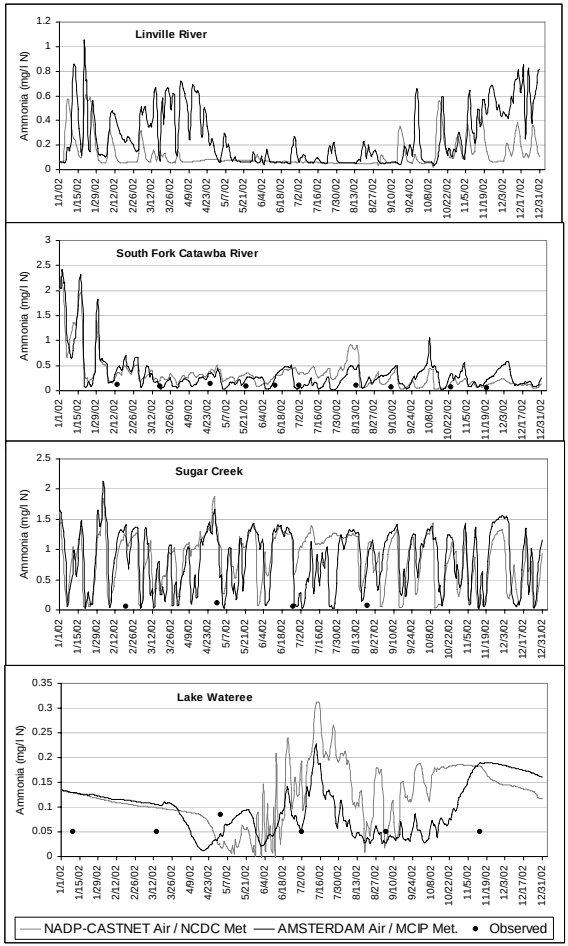

Fig. 4. Simulated ammonia concentrations in the Catawba River subwatersheds.

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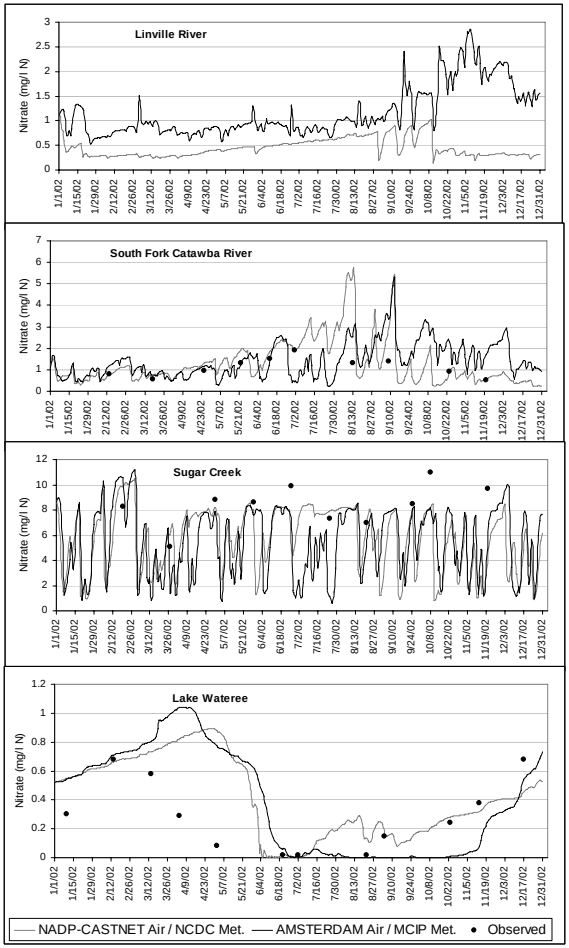

Fig. 5. Simulated nitrate concentrations in the Catawba River subwatersheds.

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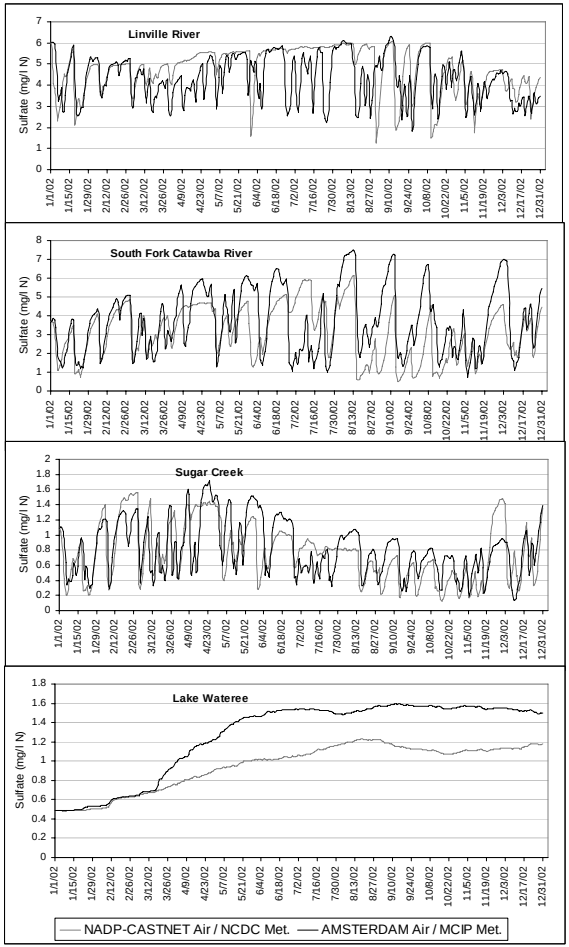

Fig. 6. Simulated sulfate concentrations in the Catawba River subwatersheds.

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