Advances in Emissions Modeling of Airborne Substances

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Abstract

The U.S. Environmental Protection Agency's Atmospheric Modeling Division is engaged in a number of research projects that are leading to advances in emissions modeling of airborne substances. Two of these projects, air quality forecast modeling and global climate change modeling, are presented in other papers at this conference. This paper briefly highlights the advances in the following areas:

(1) Ammonia emissions – development and application of an inversion technique for refining seasonal and annual estimates of ammonia
(2) Biogenic emissions – development and integration of the third generation of the Biogenic Emissions Inventory System (BEIS3)
(3) Fugitive dust emissions – development and testing of geographical databases and a dynamic algorithm for making episodic estimates of wind blown fugitive dust
(4) Sea salt emissions – development of an algorithm for estimating emissions originating from oceans
(5) SMOKE – support and refinements to the Sparse Matrix Operational Kernel Emissions (SMOKE) modeling system
(6) Wildfire and prescribed burn emissions – collaboration with the National Park Service on development of the Community Smoke Emissions Model (CSEM)

Introduction

Since the 1950s, the primary mission of the Atmospheric Modeling Division has been to develop and evaluate air quality simulation models. While the Division has traditionally focused its research on the meteorological aspects of these models, this focus has expanded in recent years to include emission processors, a critical but an inaccurate component of air quality modeling. The need for emissions modeling research has been prompted by the realization that many emission processes require dynamically-responsive algorithms that account for the meteorological conditions and the need for innovative ways to evaluate emission inventories.

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This paper briefly highlights research that is being performed in six areas: (1) ammonia inverse modeling, (2) biogenic emissions modeling, (3) fugitive dust emissions, (4) sea salt emissions, (5) support for the Sparse Matrix Operational Kernel Emissions (SMOKE) system, and (6) wildfire and prescribed burn emissions.

Ammonia Inverse Modeling

Gilliland and Abbitt (2001) discuss the development of an inverse modeling method for application with regional air quality modeling. Inverse modeling is an approach that has been used in a "top-down" manner to estimate emissions for atmospheric chemical transport models. In general, this approach compares modeled and observed concentrations and applies a linear optimization technique to adjust emissions that produce model results that better compare with observations. Inverse modeling has been used for many years with global-scale models, but few studies have historically used inverse modeling with regional-scale air quality models.

Because of the large uncertainties in ammonia (NH_3) emission estimates, we are testing the use of an inverse method for estimating NH_3 emissions. Both the annual and seasonal pattern of NH_3 is uncertain, and we suspect strong seasonal variations due to the nature of the sources. NH_3 is an excellent candidate for inverse modeling, because the response of NH_4 wet concentrations to NH_3 emissions adjustments is quite linear and because the tropospheric lifetime of NH_3 is much shorter than the monthly time scales of interest. Adjustments to monthly estimates of NH_3 emissions were derived for 1990 using wet ammonium concentration data observed during the National Atmospheric Deposition Program and simulated with the Community Multiscale Air Quality (CMAQ) model. The results of Gilliland et al. (2003) suggest that strong seasonal adjustments to estimated NH_3 emissions are needed, such that NH_3 emissions during the fall and winter should be at least 75% lower than emissions during the summer. These results also suggest that the annual estimate of the 1990 National Emission Inventory (NEI) for NH_3 is too high by at least 20%. This suggestion is supported by a recent USEPA study that proposes lower emission factors for cattle and swine, two of the largest sources of NH_3 emissions in the national inventory.

Biogenic Emissions Modeling

The Biogenic Emissions Inventory System (BEIS) has been updated several times since its introduction in 1988. BEIS estimates volatile organic compound (VOC) emissions from vegetation and nitric oxide (NO) emissions from soils at a spatial resolution as fine as 1 km. BEIS3.09 is currently formally imbedded in the Sparse Matrix Operation Emission (SMOKE) modeling system (Vukovich and Pierce, 2002). However, two research versions, BEIS3.10 and BEIS3.11, have been recently developed and are undergoing tests.

Pierce et al. (2002) introduced BEIS3.10 as part of the 2002 upgrade of the CMAQ modeling system. BEIS3.10 features a 1-km vegetation database for the contiguous United States that resolves forest canopy coverage by tree species; normalized emission factors for 34 chemicals, including 14 monoterpenes and methanol; a soil nitric oxide emissions algorithm that accounts for soil moisture, crop canopy coverage, and fertilizer application; and, speciation factors for the CBIV, RADM2, and SAPRAC99 chemical mechanisms.

BEIS3.11 involves two minor revisions to the soil NO algorithm in BEIS3.10. The soil NO algorithm has been modified to more carefully distinguish between agricultural and non-agricultural land use types. Adjustments due to temperature, precipitation, fertilizer application, and crop canopy coverage are now limited to the growing season (assumed to be April 1-October 31) and are restricted to areas of agriculture as defined by the Biogenic Emissions Landuse Database. Outside of the growing season and for non-agricultural areas throughout the year, soil NO emissions are assumed to depend only on temperature and the base emission factor is limited to that for grasslands. Another revision to BEIS3.11 is to incorporate leaf shading when estimating methanol emissions from non-forested areas. This is accomplished by assigning a nominal leaf area index of 3 for non-forested areas. BEIS3.11 will be available on the EPA web site for testing at www.epa.gov/asmdnerl/biogen.html.

To better characterize vegetation cover for estimating biogenic emissions, Pierce et al. (2002) compared vegetation cover and the resulting isoprene emission estimates from three databases: (1) the North American Land Cover Characteristics (NALCC) version 2 database, (2) the Biogenic Emissions Landcover Database (BELD3), and (3) the National Land Cover Database (NLCD). The NALCC database consists of 1-km resolved land cover classes derived from Advanced Very-High Resolution Radiometer (AVHRR) satellite data (USGS, 2001). BELD3, which currently provides vegetation data to the BEIS, combines the NALCC data with U.S. Forest Service and U.S. Department of Agriculture databases so that tree and crop cover (by species) are resolved to 1 km (USEPA, 2001). The NLCD is based on Landsat-TM data and is available at ~30 m resolution (USGS, 2002). The relative distribution of forest and agriculture cover contained in the NALCC database was found to differ considerably from the two other databases across the mixed agricultural/forested region of the Tennessee Valley. Isoprene emissions were found to vary by a factor of two depending on the source of vegetation data. Caution is therefore urged when using broadly-defined vegetation classes (such as in the NALCC data) to derive biogenic emissions. Pierce et al. (2002) recommend that future work consider using more recent databases, such as the NLCD, coupled with tree species distributions to simulate other meteorologically-related processes dependent on vegetation data.

Fugitive Dust Emissions

Work on fugitive dust has been directed towards formulating a basic understanding of fugitive dust emissions and on implementing an emissions algorithm for the CMAQ modeling system. One of the first comprehensive models for estimating wind erosion dust was given by Gillette and Passi (1988) for the National Acid Precipitation Assessment Program. Gillette et al. (1992) estimated the combined emissions of dust by wind erosion and road dust emissions, and dust devils for the 48 contiguous United

States. Physical explanations for dust emissions by wind erosion were given by Gillette (1999). Gillette and Chen (2001) explained that one challenge in estimating fugitive dust and wind emitted dust emissions is the issue of "supply-limitation." Supply limitation is simply a reduction of the emitted dust for a given meteorological condition by a lack of the source of dust from the soil or road-way. In other work, a model of dust emissions by the wind was constructed for Southwest Asia by Draxler et al. (2001). In this model, soil properties were estimated from soil samples, soil maps, geomorphic maps, and photography of locations in Northern Kuwait. An algorithm specified in the paper gave emissions of dust driven by the wind. Concentrations derived from the NOAA/ARL HYSPLIT model and observed after Desert Storm showed fair agreement. A summary of the most important properties of the soil that relate to dust emissions was given by Gillette (2002); these properties include soil texture, crusting, and soil roughness.

Gillette (2001) noted that when existing algorithms for estimating fugitive dust emissions were put into transport models, predicted concentrations downwind were found to be larger than observed concentrations at locations where fugitive dust emissions were known to be important. An initial effort to reduce this discrepancy was made by Gillette (2001). His model posited that deposition close to the source accounts for much of the discrepancy. An adaptation of this model is described by He et al. (2002), who reported on the development of an algorithm to be used in the CMAQ modeling system. Most regional air quality models have either ignored emissions of windblown and fugitive dust or have treated these emissions crudely, mainly because acceptable emission processing systems have been lacking. Algorithms for simulating windblown and fugitive dust must involve complex atmospheric processes and must link to spatially and temporally variable land surfaces, soil types, and soil condition databases. Our prototype for estimating windblown dust emissions is derived from the work of Gillette (2001). It uses threshold friction velocities parameterizations and incorporates gridded databases prepared from information on soil types, surface soil moisture content, weather, vegetation type, and vegetation coverage. Due to the variability of vegetation coverage, the non-homogeneities in the distribution of wind-erodible land use types, and the interception of the uplifted dust particles by tree and vegetation canopies, numerical studies have been performed to understand the sensitivity of the algorithm to subgrid-scale variations in the distribution of wind erodible land use type and vegetative coverage within 36 km grid cells.

Model development and testing continues on the windblown dust algorithm, and efforts have been made to link the algorithm to the CMAQ modeling system. We are evaluating a prototype in CMAQ with data from a multi-day windblown dust episode during April 2001. Development and testing of a prototype version for fugitive dust is expected to continue through summer 2003, and we hope to have the algorithm implemented into CMAQ during 2004.

Sea Salt Emissions

The aerosol module within the CMAQ model needs to account for sea salt emissions over marine environments. We have examined several sea spray generation functions

(Andreas, 1998; Monahan et al., 1986; Smith and Harrison, 1998; Smith et al., 1993) to determine their relative merits and drawbacks. Functions of Smith and Harrison (1998) appear best-suited for CMAQ's modal approach to aerosol modeling, and the necessary equations to calculate sea salt emissions from these functions have been coded into a stand-alone box model for testing. These equations calculate the number, volume and mass of emissions based on vertical wind profiles and roughness length. Our tests have included the following: (1) determining appropriate wind profile functions; (2) performing sensitivity analysis with selected input terms, such as friction velocity; and, (3) determining whether equilibrium exists between the gas and aerosol phases over marine environments (Allen et al., 1989; Hildemann et al., 1984; Nenes et al., 1998; Quinn et al., 1992).

Sea salt emissions, using the Smith and Harrison (1998) functions, have been generated as a test case for a version of CMAQ that contains a sectional aerosol module. This test case is based on a 32-km gridded national domain for a 15-day period in July 1999. Generating the emissions required spatially delineating salt-water from the Biogenic Emissions Landuse Database (BELD). Preliminary analysis of the gridded emission estimates and CMAQ simulations is underway.

Support for the Sparse Matrix Operational Kernel Emissions System

Development of the Sparse Matrix Operator Emission Kernel (SMOKE) modeling system began under the sponsorship of a cooperative research agreement between the Atmospheric Modeling Division and the North Carolina Supercomputing Center. SMOKE was designed to be applicable to any pollutant, computationally efficient, and architecturally flexible relative to other emission modeling systems. SMOKE has evolved into a community model and is being used with many air quality modeling systems. It may be downloaded at www.cmascenter/org/.

Recently, we have worked to enhance SMOKE by allowing users to group major elevated point sources by stack parameters, emissions, emission rank, plant identification number, source identification number, and plume rise (Benjey et al. 2001). We have also fixed a number of minor software "bugs" and installed a new version of BEIS (see the Biogenic Emissions section). Current efforts include installing a capability to model emissions of blowing dust and wildfires, and using alternative land cover data. We are collaborating with EPA's Office of Air Quality Planning and Standards to define a methodology to provide toxic emissions for CMAQ. The initial implementation of toxic emissions in SMOKE is limited to mobile sources using the Carbon Bond 4 mechanism, although application of the complete National Toxic Emission Inventory is planned in the near future (Strum et al., 2003). Future work will eventually combine the criteria and toxic emission inventories.

As with other emissions modeling systems, gridding raw emissions data is a challenge when running SMOKE. This function was previously accomplished by SMOKE Tool, which has been phased out along with the old Models-3 modeling framework and graphical interface (Novak et al., 1998). The core Models-3 modeling components

(CMAQ, MCIP, SMOKE) are often run independently and are unaffected by the phase-out of the old framework and interface. SMOKE Tool was used to define major elevated point sources and to grid emission data and related spatial surrogates. Point source definition is now done within SMOKE and gridding of the raw input data may be accomplished with a new Spatial Allocator tool from the Multimedia Modeling System (MIMS) (Fine et al., 2002). Spatial Allocator may be downloaded from www.epa.gov/AMD/mims/software/spatial_allocator.html. Unlike SMOKE Tool, the Spatial Allocator does not require the use of expensive SAS or Arc/Info software licenses. Finally, SMOKE can be run either independently using scripts or with the new MIMS graphical interface.

Wildfire and Prescribed Burn Emissions

In collaboration with the National Park Service and the Cooperative Institute for Research in the Atmosphere, a stand-alone emissions processor is being developed that will simulate smoke emissions from fires (prescribed and wildfires) in the CMAQ modeling system. Our goal is to build a tool with the following characteristics: (1) horizontal scale from regional to national with grid resolutions ranging from 1 to 36 km; (2) temporal resolution from hourly to multi-year; (3) chemical speciation to include criteria pollutants and their precursors; and, (4) an accuracy equivalent to other emissions estimates. The prototype, Community Smoke Emission Model (CSEM), consists of processors based on algorithms developed primarily by the US Forest Service (USFS).

These processors are designed to accomplish the following tasks:

(1) Identify fire boundaries on an hourly or daily basis from various geographical data sources. The National Fire Occurrence database, with a 1 km resolution, includes most fires for the period 1986 – 1996 and is being used in the CSEM prototype.

(2) Determine fuel loadings from fuel models that relate vegetation coverages and fuel loading data. The CSEM prototype uses EPA vegetation maps and the USFS Risk Analyses system.

(3) Compute the fuel moisture content and compare this to the fuel moisture content threshold for flammability. Fuel moisture content is being calculated from hourly temperature, relative humidity and cloudiness data from the MM5 system.

(4) Generate fires based on historical data or stochastic estimates. Historical data are derived from satellite observations or individual fire records, while stochastic estimates are based on precipitation, humidity, drought, lightning frequency, and the probability of human-induced ignitions.

(5) Determine fire behavior and biomass consumption using the CONSUME model.

(6) Compute plume rise and chemical profiles using the Emissions Processing Model or a comparable system.

Initial results from the CSEM prototype have been presented by Sestak et al. (2002), who describe the modeling prototypes from this effort and the BLUESKY project for the USFS Fire Consortia for Advanced Modeling of Meteorology and Smoke (FCAMMS). Plans are being made to evaluate CSEM with the fire emissions database for the western states being assembled by the Western Regional Air Partners' Fire Emissions Forum. Other plans are being developed by the USFS to integrate CSEM into SMOKE, to use CSEM with the CMAQ model, and to distribute CSEM via the CMAS website.

Summary

Within the Atmospheric Modeling Division, emissions modeling research is advancing in two areas. The first area features the development of innovative techniques such as inverse modeling to evaluate emissions. Inverse modeling offers tremendous potential and is leading to better seasonal profiles of ammonia emissions. The second area includes the development and evaluation of stand-alone processors that account for meteorology and simulate dynamically-varying emissions. With investment of resources in these two areas, we can improve the estimation of emissions of airborne substances.

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ADDRESSES

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