RECENT ADVANCES IN THE MODELING OF AIRBORNE SUBSTANCES

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1. 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. This paper briefly highlights new advances in the following areas since Pierce et. al., (2003):

i. Biogenic emissions – development and integration of the third generation of the Biogenic Emissions Inventory System (BEIS3)

ii. Fugitive dust emissions – development and testing of geographical databases and a dynamic algorithm for making episodic estimates of wind blown fugitive dust and unpaved road dust

iii. Air Quality Forecasting – creation of an emissions processing system for an air quality forecasting system at the National Center for Environmental Prediction (NCEP)

2. 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

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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 is available on the EPA web site for testing at http://www.epa.gov/asmdnerl/biogen.html.

A comparison of BEIS3.09 (the current version in SMOKE) and BEIS3.11 (the latest research version) for a 36 km annual simulation indicates important temporal and spatial differences in the total nitric oxide (NO) emissions from soils as a result of the algorithmic changes between these two versions of BEIS. Differences in BEIS estimates for volatile organic compound (VOC) emissions are not as significant.

3. 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.

Toward this goal, work is being done to more accurately estimate fugitive dust emissions from unpaved roads. Emissions inventory estimation methods do not accurately account for fugitive dust from unpaved roads. Our future work is to develop an algorithm for simulating fugitive dust from unpaved roads by incorporating meteorological variables such as rainfall, humidity, and soil conditions with spatially variable land surfaces, soil types, and soil condition databases. The interception of the uplifted dust particles by tree and vegetation canopies will be included within the algorithm and will be similar to the transport method described in He et. al. (2002). This algorithm will use activity data of vehicles on unpaved roads with meteorological information from a mesoscale model to create hourly, gridded fugitive dust emissions from unpaved roads.

4. AIR QUALITY FORECASTING

The creation of emission data for an air quality forecasting model requires the efficient and accurate estimation of temporal and spatial variations in emission sources of ozone precursors. To achieve this goal, the existing emission inventory preparation and processing systems need to be streamlined and modified. The critical emission precursor pollutants for ozone are volatile organic compounds (VOCs), nitric oxides (NOx), and carbon monoxide (CO). The spatial variability and temporal behavior of these compounds are influenced both by meteorological conditions and by anthropogenic activities. The key complexities in the simulation of the temporal and spatial variations of these compounds that are to be examined are the biogenic sources and the on-road mobile sources. The processing of the emission for biogenic sources can be streamlined by linking the preparation of meteorological output fields for the air quality chemistry model with the calculation of biogenic emissions. The processing of temperature-dependent emissions for mobile sources can be streamlined by using the MOBILE5B (or MOBILE6) model to create simple temperature regressions to apply to normalized emission data prior to the actual forecast. The temperature/emission relationship can then be used in a very efficient calculation for the actual emission calculation, Pouliot and Pierce (2003).

Results from this streamlined approach used operationally during the summer of 2003 show that this approach created emission inputs for the air quality model as consistent with a typical non-operational approach.

5. SUMMARY

Within the Atmospheric Modeling Division, emissions modeling research is advancing in the development and evaluation of stand-alone processors that account for meteorology and simulate dynamically-varying emissions. With investment of resources in this direction, we can improve the estimation of emissions of airborne substances.

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Disclaimer and Acknowledgements

This paper has been reviewed in accordance with the U.S. Environmental Protection Agency’s peer and administrative review policies. Mention of products or trade names does not constitute endorsement or recommendation of their use.