The Implementation of BEIS3 within the SMOKE modeling framework

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ABSTRACT

The Biogenic Emissions Inventory System version 3 (BEIS3) is being developed within the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system. A general overview of the BEIS3 model is discussed. The new input data and science algorithms implemented are summarized. The new input data includes recent land use data at 1-kilometer resolution and updated emission factors. Science algorithms to be included in future versions of BEIS3 will be mentioned. Some of these upcoming updates to BEIS3 include more detailed speciation of emissions, a new method for calculating nitric oxide emissions from soils, and a method for introducing some seasonality to the biogenic emissions through leaf age.

A BEIS3 prototype has been applied in a variety of urban and regional scale modeling applications to study its effect on photochemical modeling results. The paper will briefly discuss preliminary results and issues encountered during these model applications. Finally, this paper will discuss future plans for further improving the SMOKE-BEIS3 modeling system.

INTRODUCTION

The Sparse Matrix Operator Kernel Emissions (SMOKE)[1] model was developed to demonstrate using matrix-vector multiplication for efficient emissions processing. It reproduces the core functions of emissions processing (i.e., spatial allocation, temporal allocation, chemical speciation, and growth and control of inventory emissions). The SMOKE modeling system produced significant reductions in computing time and disk space usage[2], which is a leading factor for its implementation within the EPA Models-3 framework.

The Biogenic Emissions Inventory System (BEIS) family of models estimates emissions of Volatile Organic Compounds (VOC) that are the result of biological activity from land-based vegetative species and nitric oxide emissions that is the result of microbial activity from certain soil types [3,4]. SMOKE version 1.3 includes the Urban Airshed Model - Biogenic Emissions Inventory System (UAM-BEIS2) [5] with some modifications. The modifications to UAM-BEIS2 made in SMOKE-BEIS2 consist of (1) the correction of an error found in UAM-BEIS2, (2) updated photosynthetically active radiation (PAR) parameterization[6], and (3) conforming to the SMOKE coding standards. This paper focuses on the issues encounter during the implementation of EPA's third version of the Biogenic Emissions Inventory System [7] within the SMOKE modeling system. The first prototype, BEISv3.09, will be the primary focus with additional discussion of implementation of new algorithms in future BEIS3 prototype modeling

systems.

SMOKE-BEIS3 OVERVIEW

The types of input data used in BEISv3.09 are similar to the types used in BEIS2 models. The seven primary inputs to BEIS3 models are:

- Spatially and temporally resolved meteorological data including temperatures, solar radiation and surface pressures

- Spatially resolved, species-specific vegetation

- Species-specific biogenic emissions factors (including a winter adjustment)

- Species-specific leaf area indices (LAI)

- Chemical speciation profiles

BEISv3.09 typically uses meteorological data from the Penn State/National Center for Atmospheric Research Mesoscale Modeling System, version 1 (MM5) [8.] However, BEISv3.09 can take any meteorological data as long as it's in network Common Data Format (netCDF) [9]. BEISv3.09 uses the incoming shortwave radiation to estimate the amount of PAR available in the plant canopy.

One of the most important changes included in the BEIS3 modeling system is the use of the Biogenic Emissions Landcover Database version 3 (BELD3) [10]. The BELD3 consists of 1km horizontal resolution for 230 different land use types. The previous version, BELD2, was used in most BEIS2 applications and consisted of mainly county level land use of up to 156 different land use types. BELD3 combines the spatial resolution available from the U.S. Geological Survey (USGS) 1-km data with the detailed tree and crop species information available in county-level forest and agricultural datasets. The BELD3 data is aggregated and/or interpolated to the desired modeling domain and resolution and the land use data input into BEISv3.09 must be in netCDF. The BELD3 dataset format is available in ASCII format and EPA-Models3 framework does include tools to generate land use data in netCDF for use in BEISv3.09. MCNC has also successfully developed tools to convert BELD3 ASCII data into netCDF for input into BEISv3.09.

Emission factors in BEISv3.09 consist of isoprene, monoterpene, nitrogen oxide and other VOC factors for all BELD3 land use types. The emissions factors are the flux-rate that each species emits under standard environmental conditions (i.e. 30ºC and 1000 umol$\cdot$ m$^{-2}\cdot$ s^{-1} PAR for isoprene and 30ºC for monoterpenes, other VOCs, and NO). The emissions factors are stored in an ASCII file. This emission factors file also includes a winter adjustment factor and a leaf area index (LAI) for each land use type. Leaf area index (LAI) is defined as the total one-sided, or one half of the total all-sided, green leaf area per unit ground surface area[11]. In BEIS3, LAI is used to adjust the isoprene emissions for the effects of PAR penetrating through the leaf canopy.

The SMOKE-BEISv3.09 modeling system is a two-step process. In step one, the land use data and emissions factors file are input into a program called *normbeis3*. Figure 1

illustrates the data flows for the *normbeis3* program. The *normbeis3* program estimates normalized emissions (at 30°C and 1000 umol· $m^{-2}·s^{-1}$ PAR environmental conditions) by multiplying the emissions factor by the appropriate land use for each grid cell. These biogenic emissions data are reported in grams of Carbon or grams of Nitrogen per hour. An average LAI for each grid cell is also calculated in *normbeis3*.
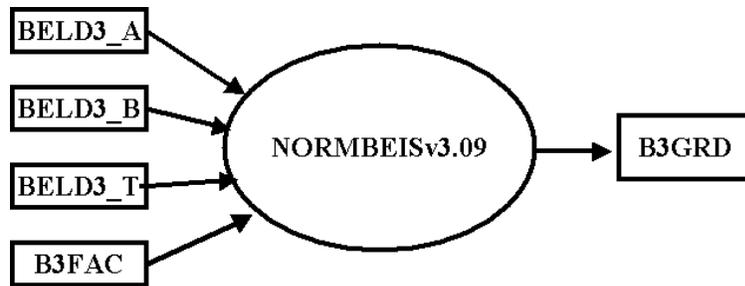
Figure 1. The program *normbeis3* input data flows.

The next program a user must execute is called *beis3*. The input data for this program consist of the meteorological data, speciation profiles, and the normalize emissions generated after the execution of *normbeis3*. The program *beis3* data flows are show in Figure 2. The speciation profiles (GSPRO) are used to allocate other VOC and monoterpene emissions to species recognized by the chemistry mechanism in the desired air quality model. The BEISv3.09 currently supports speciation of emissions for the Carbon Bond IV[12] and Regional Acid Deposition Model version 2 (RADM2)[13] chemical mechanisms.
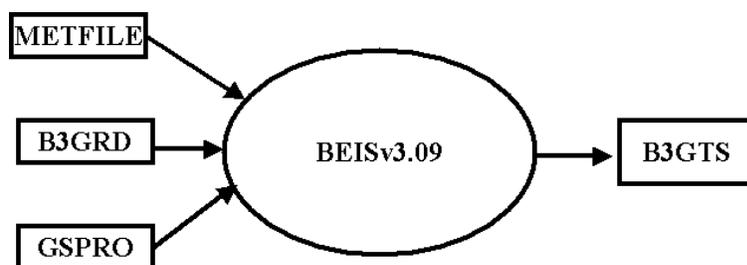
Figure 2. The program *beis3* input data flows

The output from *beis3* is gridded, speciated and temporally allocated emissions. The user can assign the units for the output emissions as gram-moles per hour or gram-moles per second. The output is in netCDF and can be input into the Multi-scale Air Quality Simulation Platform (MAQSIP) [12] and Community Multi-scale Air Quality (CMAQ) [14] modeling systems. SMOKE also has a conversion program that will convert the netCDF BEIS3 output files into a binary format recognized by the Comprehensive Air Quality Model with extensions (CAMx) [15], UAM and Regional Modeling System for Aerosols and Deposition (REMSAD) [16] models.

SOFTWARE BACKGROUND

The implementation of BEIS3 science into SMOKE followed the strict SMOKE coding guidelines[17]. These guidelines included using the FORTRAN90 computer language and the Input/Output Applications Programming Interface (I/OAPI) [18]. BEIS3 will also be able to take advantage of library routines within the SMOKE modeling system. Some SMOKE-BEIS2 routines were used in BEIS3 because some input/output methods in these models are similar. BEISv3.09 has been tested on several different UNIX platforms including SGI IRIX6 and Sun OS5.

APPLICATIONS

The BEISv3.09 modeling system has been applied in many regions in the United States. The regional applications include a northeastern United States CMAQ application, an eastern United States MAQSIP application, and a western United States UAM-V application. These applications have been valuable in the early assessment of BEISv3.09. Figure 3 illustrates the total isoprene emissions in North Carolina for a 10-day period in 1996. For this particular episode, daily summed isoprene emissions

increased 5-10% in BEIS3 when compared to BEIS2 results. Similar comparisons are still being carried out for the other regional applications and each application has and will improve future versions of BEIS3.
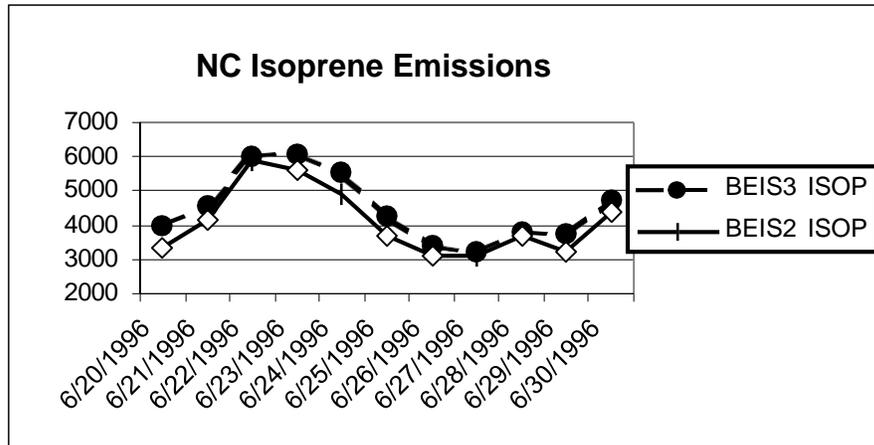
NC Isoprene Emissions

Figure 3. North Carolina isoprene emissions (in tons) for June 20-30, 1996.

CONCLUSIONS AND FUTURE WORK

The next generation of biogenic emissions modeling systems, BEIS3, has been incorporated within the SMOKE modeling system. The input data includes meteorological data, emissions factors, chemical speciation profiles, and 1-km horizontal resolution land use. The results from the SMOKE-BEIS3 model are available in various formats for use in most commonly used air quality models. The SMOKE-BEIS3 has been applied for a variety of regions and assessment of the model is still on going.

Science updates to be included in future versions of BEIS3 are already being tested. These updates will include more detailed speciation where emissions will consist of 34 different chemical compounds instead of just the nitric oxide, isoprene, monoterpenes and other VOCs. Other updates will include a nitric oxide algorithm to include soil moisture effects, chemical speciation for other chemical mechanisms, and a leaf age algorithm. These updates will be implemented within the SMOKE modeling system and documentation on the BEIS3 modeling system will be included in future SMOKE user's manuals.

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KEYWORD

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BEIS
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