APPENDIX D

BASE CASE MODELING EMISSIONS INVENTORY DEVELOPMENT

DALLAS/FORT WORTH ATTAINMENT DEMONSTRATION

APRIL 2000 REVISION

Introduction

This report supplements information provided in Appendix D of the State Implementation Plan revision dated October 21, 1998 and submitted to the EPA on March 18, 1999. Specifically, this supplement addresses the development of revised biogenic emission estimates used in the Base 5 base case, and also in the 2007d future case and control strategy D30.

D.1 Revised biogenic emissions modeling for the Dallas-Fort Worth area

D.1.1 New biogenic emissions model

TNRCC recently contracted with Environ, the University of Texas, and scientists from the National Center for Atmospheric Research (NCAR) to develop a biogenics emissions model that incorporates the latest findings in the field. This was necessary for several reasons:

- Alex Guenther of NCAR and other scientists have determined that the algorithms of BEIS2, the currently-used biogenics model, have several errors. Specifically, the calculation of solar zenith angle, the distribution of leaf mass through the plant canopy, and the coefficients that control the amount of sunlight that penetrates the plant canopy are incorrect (Guenther et al., 1998).

- Several significant recent findings in the field of biogenic emissions estimation have not yet been incorporated into any biogenic emissions model. These effects include the variation of emissions with leaf maturity (Monson et al., 1994; Geron et al., 1997; Goldstein et al., 1998), the variation of leaf emission rate among leaves that emerge in different parts of the canopy (Harley et al., 1996, 1997), and improved speciation of VOCs (Guenther et al., 1998).

- At one time, the biogenic modeling needs of TNRCC could be met by the biogenics processor of EMS-95, BIOME (Wilkinson and Emigh, 1995). This model was state-of-the-science between 1993-1998, and was used to model biogenic emissions in photochemical modeling conducted for the Houston-Galveston, Beaumont-Port Arthur, and Dallas-Fort Worth ozone nonattainment areas. However, the version of the BIOME model previously used at TNRCC was cumbersome to operate, was not particularly efficient, and lacked the flexibility needed for easily running sensitivity analyses. The TNRCC required a biogenic emissions modeling system which was easier to use, more efficient, and more flexible than BIOME.

- New land use data has been developed for the state of Texas and the surrounding states. First, recent work by researchers at the University of Texas has led to the creation of an improved land use and tree distribution map for the entire state of Texas. Second, EPA and its contractors have revised and improved the resolution of the nationwide BELD database, and have released it as BELD3 (Kinnee et al., 1997). Finally, researchers at the University of Monterrey, Mexico, and Georgia Tech have developed a land use database for the northern states of Mexico. These new databases have been consolidated into a single database, which has allowed TNRCC to create a consolidated biogenics inventory, rather than a patchwork inventory as used in previous modeling exercises. In earlier DFW modeling, the BIOME model was used in the core domain, and BEIS2 was used in the regional domain. The land use databases also differed between the core and regional domains. Now that a comprehensive land use database has been assembled for all of

Texas and the surrounding states, the same model and land use data can be used throughout all domains.

- There are indications that both BIOME and BEIS2 generate too much biogenic VOC. Environ completed a study in 1997, "Comparison of OTAG UAM-V/BEIS2 Modeling Results with Ambient Isoprene and Other Related Species Concentrations" (Morris et al., 1997), which presented strong evidence that using the BEIS2 biogenic emissions model resulted in higher predicted isoprene concentrations than are generally observed. Morris et al. showed that the effect was widespread throughout the OTAG domain, suggesting that local effects were unlikely to explain the disagreement, and that the BEIS2 model was probably responsible for the discrepancy. Internal studies by the TNRCC have also shown that ambient isoprene concentrations in Texas are often much lower than BIOME/CAMx-modeled isoprene concentrations, suggesting that there was also a positive bias in the amount of isoprene emissions predicted by BIOME.

- EPA's development of an updated biogenics model, BEIS3, has been postponed. BEIS3 will eventually incorporate the innovations described above, but is not currently available. TNRCC wanted to improve its biogenic emissions modeling in time to incorporate it into the new ozone modeling for Dallas-Fort Worth.

Therefore, to take advantage of new findings and data, to correct errors in the older models, and to improve the isoprene performance of the photochemical modeling, TNRCC sought the development of a new biogenics model.

The prototype of the new biogenics model was GloBEIS (Guenther, 1997), a biogenics model created for a variety of research applications. This model formed the foundation for the new model developed especially for TNRCC by Environ and Dr. Guenther. Dr. Guenther was also primarily responsible for development of the algorithms that govern BEIS2 (Guenther et al., 1993; Guenther et al., 1994; Geron et al., 1994). GloBEIS, and its revision GloBEIS2, are written in Visual Basic, and operate within a Microsoft® Access environment.

All the possible innovations that could have been included in the model were divided into three groups:

1. Corrections of errors in BEIS2: solar zenith angle calculation, Beer's law correction (i.e., correction of the canopy light extinction model), revised vertical leaf mass distribution;

2. Innovations that account for well-quantified and frequently observed effects: variation of emission rates with leaf maturity, variation of leaf emission rate among leaves that emerge in different parts of the canopy, revision of the speciation profiles to account for more compounds (such as methyl butenol, hexenal, and other newly quantified biogenic VOCs), addition of emission factors for more plant genera, improved emission factors for some genera;

3. Innovations that account for possible but poorly-quantified effects: dependence of emission rate upon antecedent temperature and moisture, new leaf energy balance model, escape efficiency of emitted VOCs from canopy.

Innovations in the first two categories were included in GloBEIS2; those in the last category were not included.

D.1.2 Results

Table D.1-1 shows a county-by-county summary of isoprene emissions generated with GloBEIS, and for July 3, 1996, a comparison of biogenic emissions generated using GloBEIS and with BEIS-2 and BIOME

Table D.1-1. Biogenic isoprene emissions for primary episode days, as calculated by GloBEIS2						
	Emissions by county (tons/day)					
Date	Dallas	Tarrant	Denton	Collin	Total DFW	Core domain total
6/21/95	40	53	50	16	160	3200
6/22/95	43	57	54	18	171	3453
7/3/96	56	74	71	22	225	4386
Isoprene Emissions calculated with other biogenic models, using same meteorological data (these data were not used in the current photochemical modeling; they are provided only for comparison):						
BEIS2 (7/3/96)	78	106	100	31	315	6358
BIOME (7/3/96)	72	119	201	28	421	8745

Figures D.1-1 and D.1-2 show core domain tileplots of biogenic isoprene emissions for BIOME and GloBEIS2. It should be noted that although both of these model exercises used the same temperature and solar radiation files, the land use files for the core domain are slightly different. The GloBEIS2 land use differs in the agricultural areas, where a different methodology was used in developing the agricultural land use and plant distribution information (Yarwood et al., 1999). Specifically, it was no longer assumed that the agricultural areas contained only crop species. The Land Cover Characteristics (LCC) database, developed by the U.S. Geological Survey from Advanced Very High Resolution Radiometer (AVHRR) data, was used to distinguish pure cropland from rangeland, and from crops mixed with forests, wetlands, etc. The result is that for agricultural areas such as Collin county, emissions increase or remain about the same, because areas formerly assumed to be covered with only crops now are covered with a more realistic mixture of crops and patches of trees.

Areas with dense forest have sharp decreases in emissions. This is expected, since the new model simulates sunlight penetration of the canopy in a more accurate manner. The older models allowed too much sunlight to enter the canopy, and thus had large emissions from leaves in the lowest layers. Correction of this error leads to significant decreases in emissions in areas with dense oak forests, such as in parts of Ellis and Navarro counties.

Table D.1-2 shows the change in both isoprene and total biogenic hydrocarbon emissions for the 16 km. × 16 km. East Texas modeling subdomain as a function of adopting GloBEIS.

Table D.1-2 Biogenic emissions for the East Texas domain, July 3, 1996, 16 x 16 km grid cells.			
	Isoprene Emissions (tons/day)	CB-IV Hydrocarbon Emissions (tons/day)	Isoprene as a Percentage of Total Hydrocarbons
GloBEIS2	19,460	27,660	70.3%
BIOME + BEIS2	24,330	31,850	76.4%
Percentage change in emissions in shifting from BIOME + BEIS2 to GloBEIS2	-20%	-13%	

Figures D.1-3 and D.1-4 show the combined effects of improving the land use data and switching to GloBEIS2. In the previous modeling, biogenic emissions were calculated in the core domain with BIOME, using the core domain land use database (97LULC) developed especially for DFW modeling by Environ and UT (Yarwood et al., 1997). For the regional domain, however, TNRCC had to rely upon the default BELD2 database for land use coverage, and therefore had to use BEIS2 as the biogenic emissions model. As Figure D.1-3 clearly shows, these two modeling regimes did not yield similar results in the western part of the domain; there is a very distinct discontinuity in emissions estimates. This is due primarily to inaccuracies in the BELD2 database. Approximately west of 97° longitude, the BELD2 database relies almost completely upon satellite data to assign land use categories; very little ground-truthing was done to check the land use assignments. Hence, it does not correctly assign the land cover classification for areas in Texas roughly west of 97° longitude. The disagreement between the BELD2 database and the 97LULC database results in an abrupt transition when the core domain emissions are overlaid upon the regional domain emissions. While this discontinuity was not very realistic, more refined land use data were not available at the time to correct this discontinuity, and so it remained in the modeling. In the newest round of modeling (see Figure D.1-4), however, the consolidated land use database developed for the State of Texas by UT (99LULC) eliminates this discontinuity by more accurately determining the land use for the western parts of the domain. The new LULC assignments, based upon Texas Parks and Wildlife data and ground surveys by UT, properly identify these areas as mixed oak and juniper woodlands.

Table D.1-3 shows that overall isoprene emissions decrease when GloBEIS2 replaces the previous biogenics emissions modeling. Figure D.1-4 shows, however, that isoprene emissions in the western part of the east Texas domain increase due to better characterization of land use. GloBEIS2 has a slightly different VOC speciation as well; the percentage of VOC emissions comprised by isoprene decreases slightly.

Table D.1-3. Daily Biogenic VOC emissions for DFW Nonattainment Counties, Calculated by GloBEIS2.		
Date	Isoprene (tons/day)	Total Hydrocarbons (tons/day)
6/18/95	131	151
6/19/95	138	158
6/20/95	149	170
6/21/95	160	183
6/22/95	171	195
6/30/96	211	242
7/1/96	213	245
7/2/96	222	256
7/3/96	225	258
7/4/96	212	243

GloBEIS2 calculates emissions for three categories of hydrocarbon (isoprene, monoterpenes, and other VOCs), carbon monoxide, and nitric oxide. Table D.1-4 lists the compounds that were used to create CB-IV conversion factors for monoterpenes and other VOCs. The model calculates emissions with emission factors for Total Monoterpenes and Other VOCs. The CB-IV emissions are then calculated by converting from moles of Total Monoterpenes to moles of CB-IV species, with the conversion factor based upon the list of monoterpenes in Table D.1-4. The CB-IV speciation profiles used are constant for all parts of the domain.

Table D.1-4. Chemical species used by GloBEIS2 to create Carbon Bond IV speciation profiles for monoterpenes and OVOCs.			
Terpenes	***Alcohols***	***Carbonyls***	***Olefins and paraffins***
α-pinene	methanol	acetone	ethene
β-pinene	ethanol	butanone	propene
Δ3-carene	methyl butenol	acetaldehyde	butene
sabinene	hexenol	formaldehyde	ethane
limonene		hexenal	
β-phellandrene		hexanal	
r-cymene		hexenylacetate	
myrcene		bornyl acetate	
camphene		acetic acid	
camphor		formic acid	
α-thujene			
terpinolene			
α-terpinene			
γ-terpinene			
ocimene			
1,8-cineole			
piperitone			

D.1.2 Bibliography

Guenther et al. (1993). Isoprene and monoterpene emission rate variability: model evaluations and sensitivity analyses. *JGR* 98(D7): 12,609-12,617.

Guenther et al. (1994). Natural VOC emission rate estimates for US woodland landscapes. *Atmos. Environ*. 28(6): 1197-1210.

Guenther et al., (1995). A global model of natural VOC emissions. *JGR* 100(D5): 8873-8892.

Guenther (1997). Seasonal and spatial variations in natural VOC emissions. *Ecol. Appl*. 7(1): 34-45.

Guenther et al. (1998). Natural emissions of non-methane volatile organic compounds, carbon monoxide, and oxides of nitrogen from North America. NARSTO Review Paper, April 1998.

Goldstein et al. (1998). Seasonal course of isoprene emissions from a midlatitude deciduous forest. *JGR* 103(D23): 31,0445-31,056.

Harley et al. (1996). Effects of light, temperature, and canopy position on net photosynthesis and isoprene emission from sweetgum leaves. *Tree Physiol*. 16(1-2): 25-32.

Harley et al. (1997). Environmental controls over isoprene emission in deciduous oak canopies. *Tree Physiol*. 17: 705-714.

Kinnee et al. (1997). United States land use inventory for estimating biogenic ozone precursor emissions. *Ecological Appl*. 7(1): 46-58.

Monson et al. (1994). Environmental and developmental controls over the seasonal pattern of isoprene emission from aspen leaves. *Oecologia* 99(3-4): 260-270.

Monson et al. (1995). Biological aspects of constructing VOC emission inventories. *Atmos. Environ*. 29(21): 2989-3002.

Morris et al. (1997). *Comparison of OTAG UAM-V/BEIS2 Modeling Results with Ambient Isoprene and Other Related Species Concentrations, Final Report.* Prepared for Marcel Haberstadt, American Automobile Manufacturers Association by R. Morris, K. Lee and G. Yarwood of ENVIRON International Corp., October 31, 1997.

Wilkinson and Emigh (1995). EMS-95 BIOME Model User's Guide

Yarwood et al. (1999). *Biogenic model and land use data development project, Final Report.* Prepared for Mark Estes of Texas Natural Resource Conservation Commission (TNRCC) by G. Yarwood, G. Wilson,,,, of ENVIRON International Corp., D. Allen, C. Wiedinmyer, and W. Strange of the University of Texas at Austin Chemical Engineering Department, and Alex Guenther of the National Center for Atmospheric Research (NCAR). To be completed in December 1999.

Yarwood et al. (1997). *Leaf biomass density data for north central Texas, Final Report.* Prepared for TNRCC, by G. Yarwood and K. Lee of ENVIRON International Corp., D. Allen, C. Quigley, C. Wiedinmyer, W. Strange of the UT Chemical Engineering Department, and Alex Guenther and Bill Baugh of NCAR, October 15, 1997.

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Figure D.1-1 BIOME model estimates for biogenic VOC emissions, calculated for the previous round of modeling. The DFW core emissions inventory domain is shown for July 3, 1996, at a resolution of 4x4 km.

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Figure D.1-2 GloBEIS2 model estimates for biogenic VOC emissions calculated for the current round of modeling. The DFW core emissions inventory domain is shown for July 3, 1996, at a resolution of 4x4 km.

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Figure D.1-3. BIOME and BEIS2 model estimates for biogenic isoprene emissions, July 3, 1996. There is a sharp discontinuity at the boundary of the core and regional domains due to the different land use data and different models used for the two domains. The gridcells presented in this map are 16x16 km.

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Figure D.1-4. GloBEIS2 model estimates for biogenic isoprene emissions, July 3, 1996. The discontinuity present in the earlier modeling has been eliminated. The gridcells presented in this map are 16x16 km.