APPENDIX E

Development of Revised Biogenics Emissions for the SuperCOAST Domain Using GloBEIS

Houston/Galveston Attainment Demonstration and
Post-1999 Rate-of-Progress SIP

December 2000

Revised biogenic emissions modeling for the Houston-Galveston area

Development of a 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, 1999).

- Several significant recent findings in the field of biogenic emissions estimation are not incorporated into BEIS2 or Biome. These findings include variation of emissions with leaf maturity (Monson et al., 1994; Geron et al., 1997; Goldstein et al., 1998), 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).

- 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 biogenic 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 BEIS2/UAMV-modeling 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 is 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 Houston-Galveston.

Therefore, to take advantage of new findings and data, to correct errors in the older models, and to consequently improve the isoprene performance of the photochemical modeling, TNRCC is using a new biogenics model, Globeis2.

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. In his earlier work, Dr. Guenther developed the algorithms that govern BEIS2 (Guenther et al., 1993; Guenther et al., 1994; Geron et al., 1994); his work on Globeis was an extension of that effort. Globeis and its revision Globeis2 are written in Visual Basic, and operate within a Microsoft® Access environment.

Several innovations are incorporated into this model:

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 several 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.

Although the model is capable of varying the emission rates in conjunction with the seasons, the modeling included here did not employ the seasonal variation algorithms, due to some problems with quantitatively applying them in Texas.

Table 1 presents the sources of the modeling algorithms and data used in Phases 1-3 modeling for the Houston-Galveston core domain and for the regional domain.

Table 1. Sources of biogenic modeling algorithms and data, COAST domain				
Modeling Phase	Canopy model	Emission factors	Meteorological Data	Land use data
Phase 3	Globeis2 (Yarwood et al., 1999b; Guenther et al., 2000)	Globeis2 (Yarwood et al. 1999b; Guenther et al., 2000)	National Weather Service (NWS)	Yarwood et al., 1999b
Phase 2	BIOME (Wilkinson and Emigh, 1995; Radian, 1993)	BEIS2 (Geron et al., 1994)	NWS	Yarwood et al., 1999a
Phase 1	BIOME (Wilkinson and Emigh, 1995; Radian, 1993)	BIOME (Radian and VRC, 1994)	NWS	Radian and VRC, 1994
Sources of biogenic modeling algorithms and data, regional domain excluding COAST				
Phase 3	Globeis2 (Yarwood et al. 1999b; Guenther et al., 2000)	Globeis2 (Yarwood et al. 1999b; Guenther et al., 2000)	NWS	Yarwood et al., 1999b; Kinnee et al., 1997; Mendoza-Dominguez et al., 1999
Phase 2	BEIS2 (Geron et al., 1994)	BEIS2 (Geron et al., 1994)	NWS	BELD2
Phase 1	BEIS2 (Geron et al., 1994)	BIOME (Wilkinson and Emigh, 1995; Radian, 1993)	NWS	BELD2

Globeis2 results for southeastern Texas
Table 2 presents biogenic VOC emissions estimates for each of the eight nonattainment counties.

Table 2. Biogenic emissions for primary episode days, as calculated by Globeis2									
Date	Isoprene emissions by county (tons/day)								
	Harris	Montgomery	Liberty	Chambers	Galveston	Brazoria	Fort Bend	Waller	8-county total
9/09/93	101	130	169	27	17	113	57	35	649
9/10/93	147	184	210	30	18	133	75	48	844
9/11/93	123	158	184	27	16	116	63	41	727
CB-IV hydrocarbon emissions, in tons/day, calculated for 9/10/93 using same meteorological data for all scenarios:									
Globeis Phase 3	231	342	340	52	23	159	90	73	1308
Biome Phase 2	263	363	381	85	41	240	113	85	1573
Biome Phase 1	366	367	348	77	44	123	45	78	1448

The following features are notable:

1. Day-to-day variation of isoprene emissions is large. For the entire eight-county area, isoprene emissions vary by 100-200 tons/day. In Harris County alone, during two consecutive days, isoprene emissions vary by 46 tons/day. This fluctuation is primarily due to day-to-day variations in ambient temperature.

2. Globeis2-calculated emissions of total hydrocarbons decreased by 265 tons/day compared to the emissions calculated in Phase 2, a decrease of 18%. This result is consistent with the change in canopy model algorithms between Globeis2 and BIOME. Areas with dense forest have sharp decreases in VOC emissions. This is expected, since the new model simulates sunlight penetration of the canopy more accurately than BIOME by more strongly attenuating the light that reaches the lower portions of the forest canopy. BIOME and BEIS2 allowed too much sunlight to enter the canopy, and thus overestimated emissions from leaves in the lowest layers. Correction of this error leads to significant decreases in emissions in areas with plentiful vegetation.

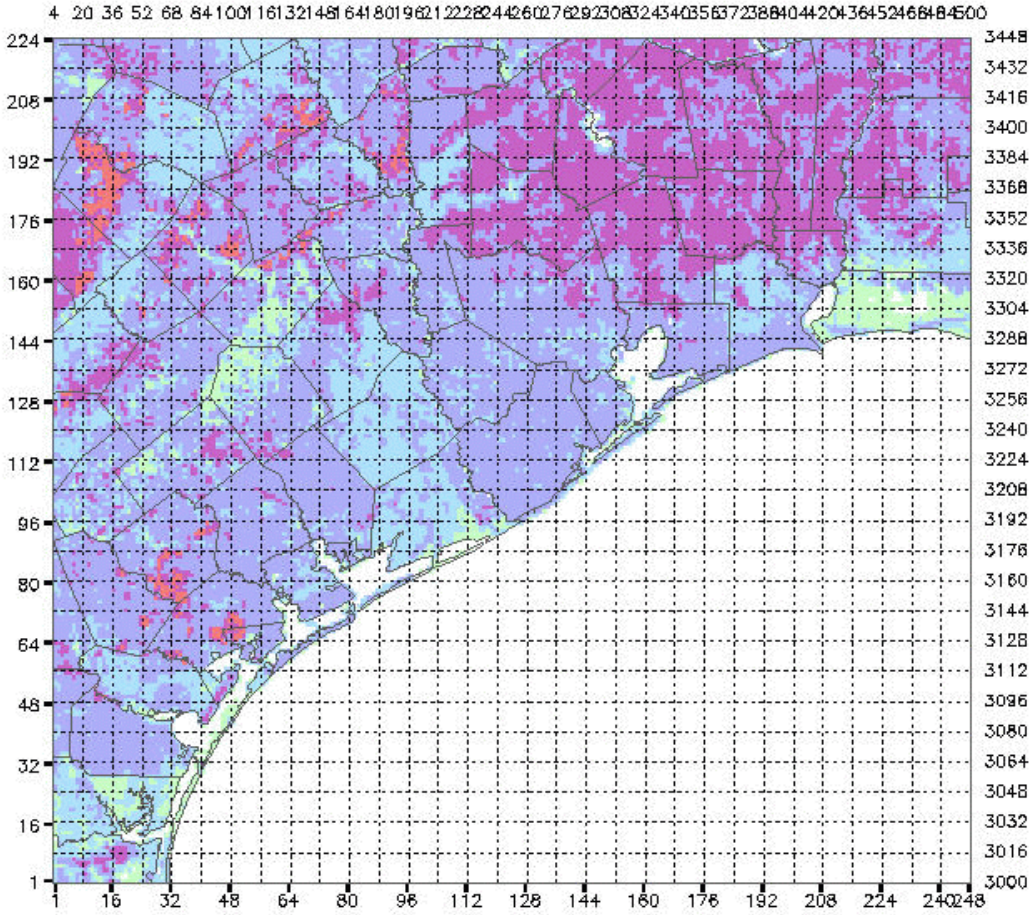
3. Four of the eight counties generate about 80% of the biogenic VOCs: Liberty, Montgomery, Harris, and Brazoria.

Figures 1 and 2 show core domain tileplots of biogenic isoprene emissions for BIOME and Globeis2.

COAST_PHASE_2 Biogenic CB-IV HC Emissions, 09/10/93

COAST 2km BIOME

(2x2 Km Grid Cells)



Emissions Plotted

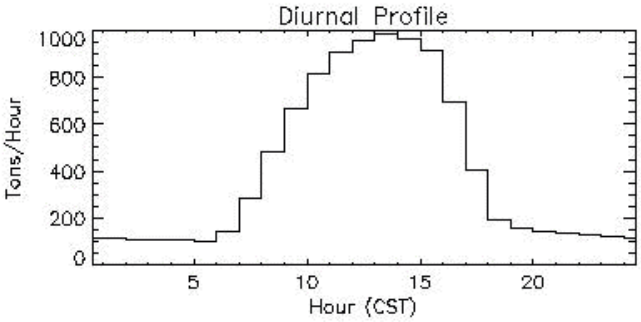
County	Tons/Day
Brazoria	240.48
Chambers	85.22
Fort Bend	112.92
Galveston	41.03
Harris	263.43
Liberty	381.56
Montgomery	363.33
Waller	85.04
HG SUBTOTAL:	1573.02
Hardin	359.27
Jefferson	120.08
Orange	100.89
BPA SUBTOTAL:	580.24
MAP TOTAL:	9734.80

Legend (Tons/Day)

< 0.00 | 0.00 – 0.01 | 0.01 – 0.10 | 0.10 – 0.50 | 0.50 – 1.00 | 1.00 – 2.00 | 2.00 – 5.00 | >= 5.00

Max Cell: 1.6 tons/day at (37, 3369)

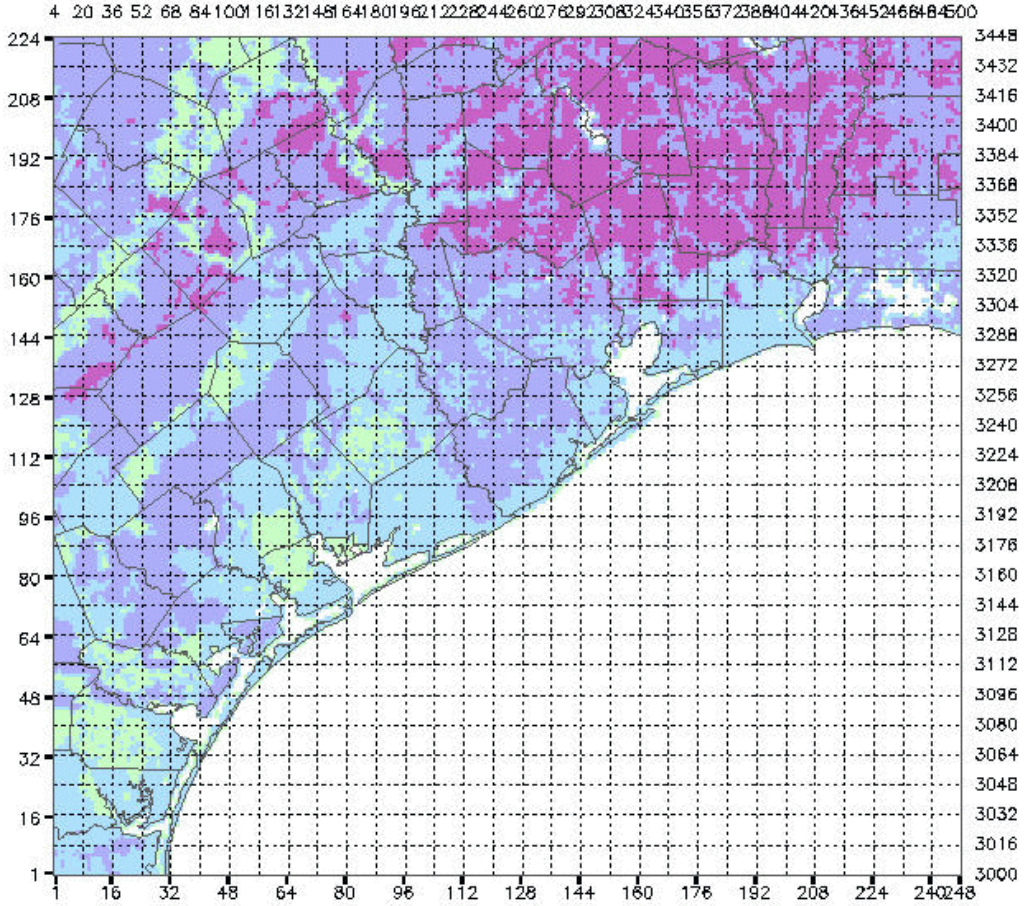
Diurnal Profile



THRCC NJE: 08/02/2000 10:33:15: /ems95_hgbpa/grid_2km/scenario/091093/alrehed/freehead_bio.091093

COAST_PHASE_3 Biogenic CB-IV HC Emissions, 09/10/93

COAST 2km Globeis
(2x2 Km Grid Cells)



THRCC MJE: 08/02/2000 10:19:53: /bforeg/globout/hgeep93/hgnoeeep930910_2km.bin

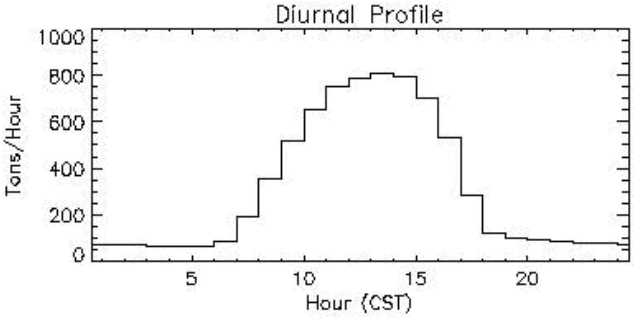
Emissions Plotted

County	Tons/Day
Brazoria	158.94
Chambers	51.75
Fort Bend	89.79
Galveston	22.72
Harris	230.69
Liberty	339.77
Montgomery	341.52
Waller	72.72
HG SUBTOTAL:	1307.89
Hardin	330.45
Jefferson	58.89
Orange	84.38
BPA SUBTOTAL:	473.71
MAP TOTAL:	7430.08

Legend (Tons/Day)

- < 0.00
- 0.00 – 0.01
- 0.01 – 0.10
- 0.10 – 0.50
- 0.50 – 1.00
- 1.00 – 2.00
- 2.00 – 5.00
- >= 5.00

Max Cell: 0.8 tons/day at (31, 3381)



Biogenic NO_x emissions estimated by Phase 3 modeling decreased slightly compared to Phase 2 estimates, due to the changes in land use data.

Table 3. Biogenic NO_x emissions for the Houston nonattainment area, September 10, 1993.	
	Nitrogen Oxide Emissions (tons/day)
Globeis2	17.8
BIOME	20.3
Percentage change in emissions in shifting from BIOME to Globeis2	-12.3%

Regional biogenic VOC and NO_X emissions estimated for Phase 3 modeling are presented in Table 4. At the regional scale, both biogenic VOC and NOX increased. The increase not only reflects the change in models but also the change in land use data (see Table 1).

Table 4. Regional domain biogenic VOC and NOX estimates for Phase 2 and Phase 3 modeling.		
	VOC (tons/day)	NOX (tons/day)
Phase 3 Globeis2	65,623	2119
Phase 2 BIOME + BEIS2	54,780	1511

Another difference between the new estimates and the old estimates is the distribution of VOCs. Previously, VOCs were apportioned among only a few Carbon Bond IV species: ISOP, PAR, OLE, ALD2, and NR. Globeis2, however, apportions VOCs more realistically to many Carbon Bond IV categories: ISOP, PAR, OLE, ALD2, XYL, FORM, ETH, MEOH, ETOH, and NR. The new speciation is based upon improved monoterpene and oxygenated hydrocarbon data (i.e., Helmig et al., 1999a, 1999b). Table 4 lists the compounds that were used to create CB-IV conversion factors for monoterpenes and other VOCs. The CB-IV speciation profiles used are constant for all parts of the domain.

Table 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	

Table 5 compares the CB-IV hydrocarbon speciation for Phase 3 Globeis2 modeling and Phase 2 Biome modeling for September 10, 1993. The main change seems to be a reapportionment from PAR to MEOH. The reactivity of the VOC mixture has probably not changed significantly from Phase 2 to Phase 3.

Table 5. CB-IV speciation of hydrocarbon emissions for September 10, 1993 in the Houston-Galveston nonattainment area, calculated Phase 3 and Phase 2 modeling.

CB-IV hydrocarbon species	Phase 3: Emissions (tons/day)	Phase 3: Percentage of total hydrocarbons	Phase 2: Emissions (tons/day)	Phase 2: Percentage of total hydrocarbons
ISOP	844	65%	1018	65%
PAR	197	15%	407	26%
OLE	67	5%	57	4%
ALD2	53	4%	91	6%
MEOH	113	9%	0	0
ETH	11	>1%	0	0
ETOH	11	>1%	0	0
FORM	3	>1%	0	0
XYL	8	>1%	0	0
CB-IV Hydrocarbon Total	1307	100%	1573	100%

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