2005 & 2006 Episodic Ozone Modeling EI Development Update

Southeast Texas Photochemical Modeling Technical Committee Meeting

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44 Pages
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Today's Presentation

- **Photochemical Model Input Requirements**
- **EI Development and Preprocessing Tools**
- **Overview of each Source Category**
- **Completed Tasks in each Source Category to Date**

Photochemical Model Inputs

In General

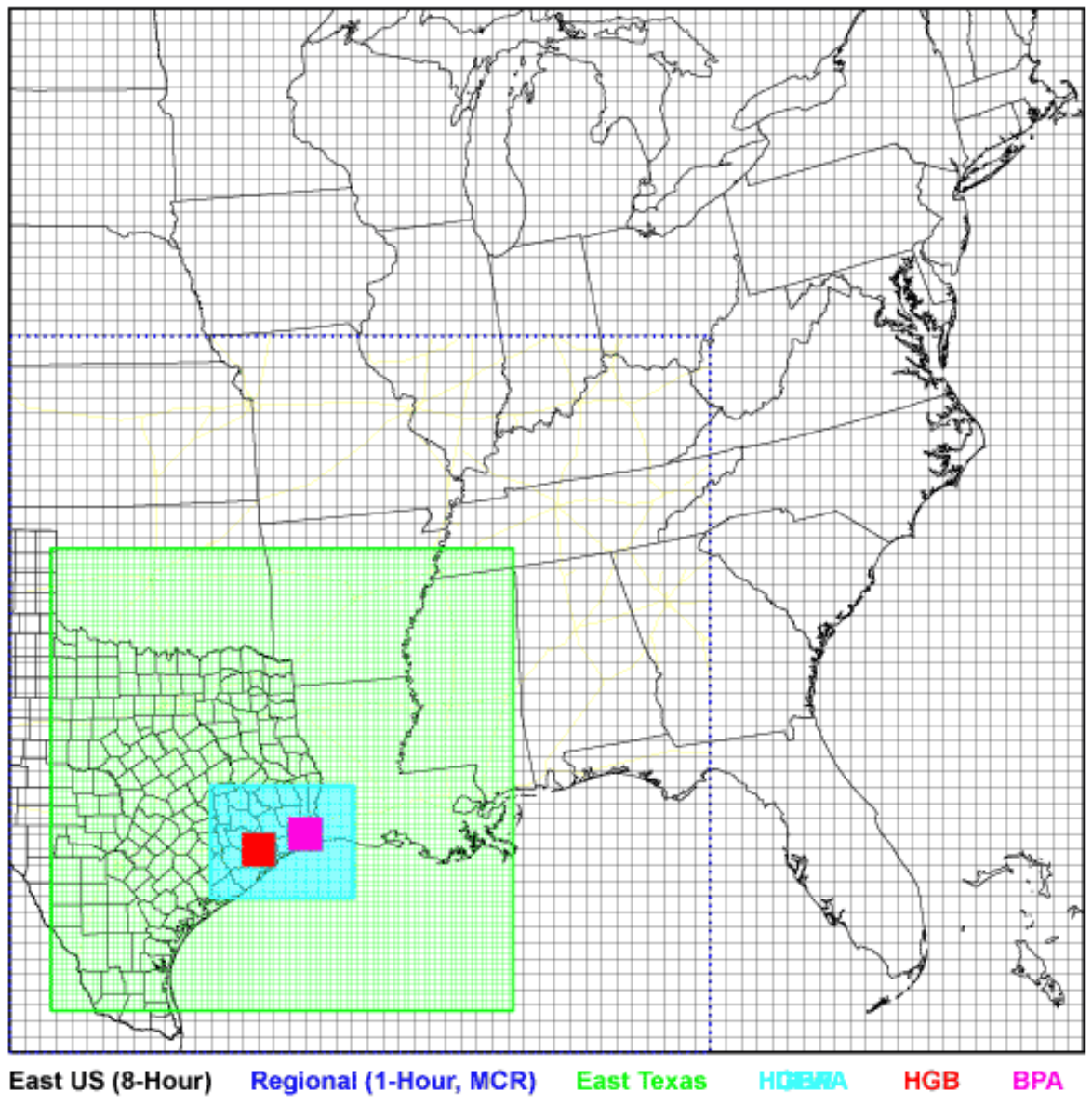
A Model by Many Other Names

- SIP Model
- Ozone Model
- Photochemical Model
- Urban Airshed Model
- Mesoscale Model
- CMAQ (Community Mesoscale Air Quality model)
- CAMx (Comprehensive Air Quality Model with extensions)

Model Input Requirements

- Domain and Episode Definitions
- Hourly Meteorological Data
- Hourly Emissions Data
  - Spatially Allocated
  - Temporally Allocated
  - Chemically Allocated (Speciated)

HGB CAMx Modeling Domain



2005 & 2006 Episodes

- Coordinated with meteorology development timeline
  - Sufficient nudging data available
  - Sufficient statistical performance
  - In likely order of met file completion:
    - 7/26 – 8/8/2005
    - 6/15 – 6/30/2005
    - 5/19 – 6/03/2005
    - 5/31 – 6/16/2006
    - 8/01 – 10/15/2006 (TexAQS II Intensive)

Modeling a Base Case

- Purpose
  - Proof the model
  - Replicate the ozone production of the historical episode
  - Provides confidence that the meteorology and the emissions are accurate enough for a future year attainment demonstration
- Judging Success
  - Does the model predict the same ozone levels that were monitored at the same location at the same time?
  - “Model Performance Evaluation”

Emissions for a Base Case

- Use highest resolution emissions data available, hierarchically
  - Most detail in the nonattainment area of interest - smallest grid size
  - Somewhat lesser amount of detail in the larger grid cells – Texas and surrounding
  - Least amount of detail in areas furthest from Texas – in the largest grid cells – “region”
- Use raw hourly where available
- Create hourly profiles otherwise (see temporal allocation)

EI Development and Preprocessing Tools

EPS

- Emissions Preprocessing System
- Improved Periodically by Environ (current version is EPS3)
- Assists with Allocation of Emissions
  - Spatially
    - Assign low-level emissions to specific grid cells
    - Elevated emissions maintain geographic locale
  - Temporally
    - Convert annual or daily emissions into hourly
  - Chemically
    - Break total VOC and NOx into species families using a chemical mechanism (CB-IV, CB05, SAPRC)

Create AFS/AMS Records

- AIRS Facility Subsystem (AFS) for Point Sources
  - One record for each Account/FIN/EPN/SCC/Pollutant combination
  - If hourly, one record for each Account/FIN/EPN/SCC/Pollutant/Hour combination (massive file sizes)
- Area and Mobile Source (AMS)
  - One record for each county/SCC/Pollutant combination
  - One record for each county/vehicle class/road type/ASC/link (also massive file sizes)
- Pollutants
  - NOx
  - VOC
  - CO

  } for O_3 chemistry
- Emission Rate
  - Annual
  - Ozone-Season Daily
  - Hourly

Example AFS Record

```
B 00 00 AC 48013 ETX   4911 10100301   0007
0001       001            S  00090100 00090101
149.83820 -1235.2500    137.2 6.098   350 36.07
28  17  28  27 24  0 7 8736 42101   0.336971
AG0007G BOILER1    STACK1     San Miguel P SAN
MIGUEL ELECTRIC COOPERATIVE IN ATASCOSA
CHRISTINE       CO

ST 05/30/2001 ARP
```

Spatial Allocation

- Surrogates for Area and Mobile (county-level allocated to more specific areas)
  - e.g., urban center, lakes, population, interstate highway
- Low-level
  - Emissions records with low plume rise (e.g. < 30m)
  - Lumped into grid cells
  - Added to all other parts of gridded EI at final EPS merge step
- Elevated
  - Modeled initially from (x,y) point of reported coordinates
  - Modeled initially from calculated plume rise height (z) in CAMx
- QA
  - Tileplots

Tileplot

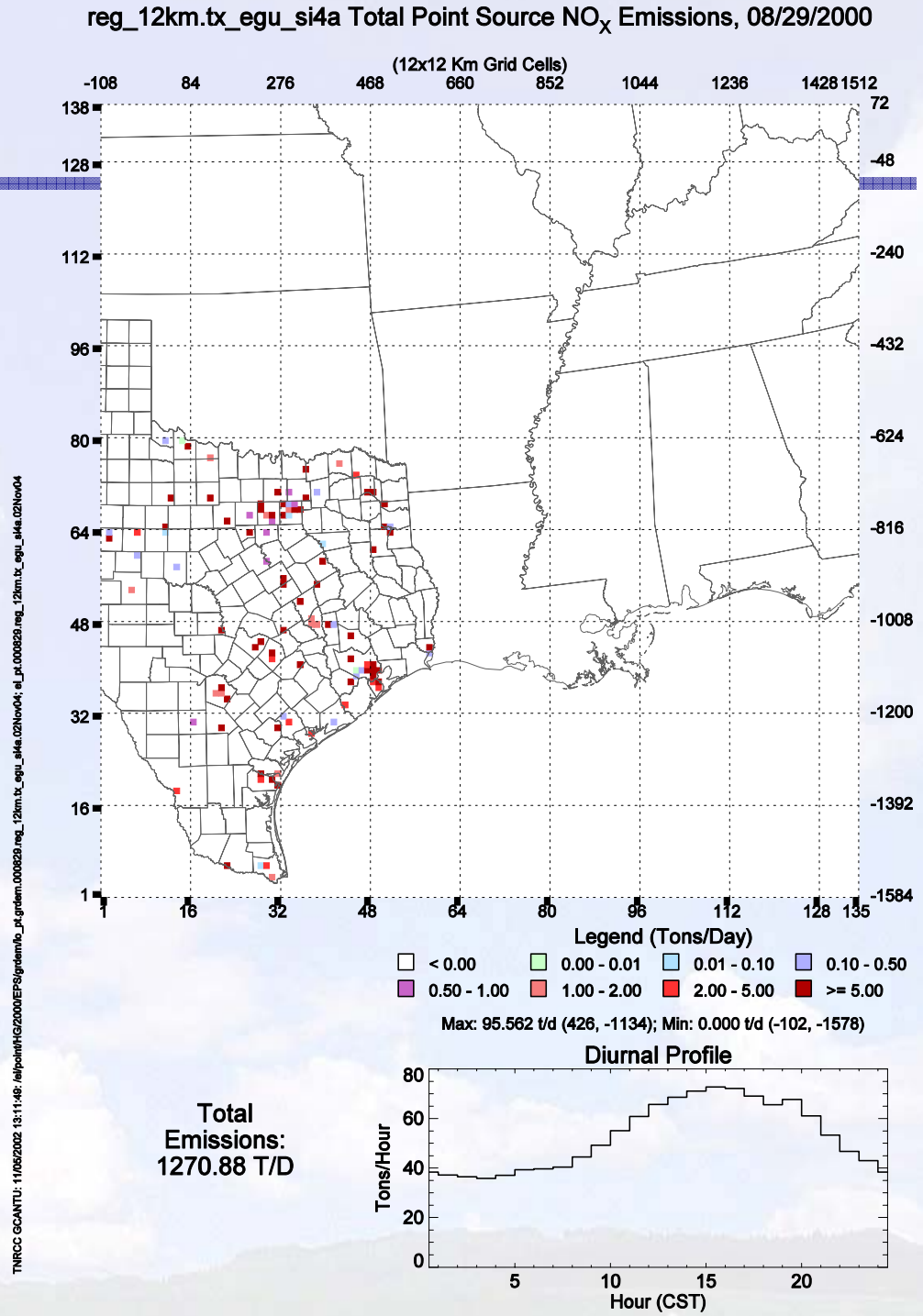
Texas

12 km grid

EGU w/ SI

NOx

8/29/2000



Temporal Allocation

- AFS/AMS records may contain
  - Seasonal (percentage of year) use of equipment
  - Annual (weeks per year) use
  - Weekly (days per week) use
  - Daily (hours per day) use
  - Start Hour (hour of day that operations start each day)
- Each record assigned a temporal profile
  - Profile is a calculated percentage of total emissions for each hour, for those hours which it operates
  - Compact method rather than 24 records for each AFS/AMS record
  - Many AFS/AMS records can share the same profile
- QA
  - Tileplots

Temporal Allocation -cont

- Or if you have access to Hour-Specific Data
  - These do not receive Temporal adjustment/profile
  - Provide for true bottom-up hourly modeled emissions
  - TxDOT, TTI Mobile Source files by county and day type (weekday, Friday, Saturday, Sunday)
  - EPA Acid Rain Program CEM for Point Source EGUs
    - Hourly data received, housed and QA'd by EPA
    - TCEQ creates xref between Acid Rain Program boiler identifiers and STARS/NEI identifiers
  - Special Inventory
    - TexAQS 2000, 2005, TexAQS II 2006
  - CCEDS events

Chemical Allocation (Speciation)

- AFS & AMS files contain only lumped VOC (total VOC)
- Break the VOC into chemical constituents
  - Based on chemical profile files, generally by SCC (EPA defaults or specific contracts to generate Texas-specific profiles)
  - Point sources are generated as point-specific or SCC-specific
- **Example: gasoline (one variety) is 35% heptane, 15% isooctane, 25% cyclopentane, 25% ethylbenzene**

Chemical Allocation (Speciation)

Sample CB-IV Representation

SPECIES	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH
ETHYLENE	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
PROPENE	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-BUTENE	2.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1,3-BUTADIENE	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PENTENE	3.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HEXENE	3.00	0.33	0.00	0.00	0.00	1.17	0.00	0.00	0.00	0.00
ISOPRENE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00

Other Tools

- SAS (file format conversion, programming, analysis, QA summaries)
- PV-Wave (visual QA Tileplot generation, programming)
- Perl Scripting (file manipulation, QA summaries)
- FORTRAN (model compiling, programming)
- GIS (surrogates, biogenics, visualization)
- MS-Access (biogenics, NEI)

Data Sources for Each Category

Overview

Sources of Point Source Modeled Data

- STARS snapshot (IEAS, Modelers)
- Special Inventory (IEAS, Modelers)
- CCEDS (OCE, Modelers)
- Acid Rain Program CEM (EPA, Modelers)
- Louisiana (LDEQ, 2004 NEI)
- Oklahoma (ODEQ, 2005 NEI)
- Offshore (MMS, 2000 GWEI)
- Regional (NEI, 2002 Final or 2002 RPO)
- Canada (Canada, 2000)
- Mexico (BRAVO, 2000)

Sources of Area and Non-road Modeled Data

- TexAER, 2002 PEI
  - Updated surveys
- NONROAD2004 model, NMIM (National Mobile Inventory Model)
- Texas ships as pseudo points
- Regional, 2002 NEI
- Offshore (MMS, 2000 GWEI)
- Canada

Onroad Mobile Sources of Modeled Data

- TCEQ Hourly Link-based contract with TTI
  - MOBILE6.2 emission rate output
  - VMT data from Travel Demand Model
- TTI Hourly county-level for Texas outside of Nonattainment area
- 2005-2006 Base Case
  - Generic Weekday (Monday – Thursday)
  - Friday
  - Saturday
  - Sunday
  - Hourly Temperature and Humidity corrections
- Regional (2002 NEI, using Texas-derived profiles)

Sources of Biogenic Modeled Data

- Land Cover & Vegetation Data
  - UT Center for Space Research has developed new data, circa 1999-2003. Uses data from Texas Forest Service's Houston Green project, USDA Forest Inventory & Analysis data, new USGS National Land Cover Data, recent satellite and aerial photography
- Temperature Data
  - Kriging of observed temperatures to generate grid cell values by day and hour
- Photosynthetically-Active Solar Radiation data
  - GOES8 satellite-derived data
- Model Used: GloBEIS3
  - Guenther, et al. & Environ, 1999

Completed EI Tasks to Date

Progress Report

EI Task Details

- EM-1
  - Obtain extracts from STARS for most recent point source emissions (e.g., 2004/2005)
  - Delay in 2005 complete data upload into STARS
  - 2004 is Complete as a placeholder/backup
  - Bonus: write more information fields from STARS into AFS files

EI Task Details -cont

- EM-2
  - Obtain extract from EPAs ARPDB for each episode for which data are available and where appropriate substitute the ARPDB data for the STARS data
  - Complete
  - Hourly ARPDB files have been generated

EI Task Details -cont

- EM-3
  - Obtain emissions events data from TCEQ databases (CCEDS & EMRS) substitute for STARS, where appropriate
  - Not readily useful:
  - EMRS does not contain FIN/EPN with which to match. EMRS does not collect more detailed info.
  - CCEDS does not contain enough temporal detail to calculate hourly emissions. The FIN-EPN-NUM field in CCEDS does not provide a clear match to an AFS/STARS record, because the reporter is not mandated to use names in STARS. Matching would be very labor-intensive, and would have to verify guess with the reporter/industry representative for QA
  - Propose to begin the process with the largest events from areas of greatest concern.

EI Task Details -cont

- EM-4
  - Substitute special hourly emissions (2005 & 2006 TexAQS II) for STARS, where appropriate.
  - HEIRS (Hourly Emissions Inventory Reporting System) data for 2005 has recently been uploaded into STARS. IEAS is working on upload of 2006 TexAQS II HEIRS data
  - 2005 HEIRS was limited to 22 accounts in Harris county, and covered May 3-7 and May 12-June 4, so may be good for only the May 20-June 5, 2005 episode
  - 2006 HEIRS should be useful for the TexAQS II intensive period of August 15-September 15
  - Researched, but no records substituted until 2005 STARS Extract is available

EI Task Details -cont

- EM-5
  - Obtain the 2002 NEI for states outside Texas, substitute ARPDB data, where appropriate and forecast other data as appropriate for the episodes (i.e., 2005/2006).
  - The 2002 NEI includes on- & non-road and area source, as well as point source emissions
  - Gathered and generally converted, but not QA'd for points
  - Points also comparing the 2002 CENRAP/RPO, which is supposed to be better QA'd, but may have its own issues. Doing comparisons now.
  - Points have gathered 2005 NEI from OK, will try to gather 2004 NEI from LA and AR
  - Completed for area, non-road, and mobile

EI Task Details -cont

- EM-6
  - Obtain the most recent emissions updates for the MMS off-shore, Canada & Mexico and forecast as appropriate for the episodes (i.e., 2005/2006)
  - Include points, on- & non-road and area sources
  - No updates to offshore (MMS 2000 GWEI)
  - No updates to Canada (security issues) or Mexico (2000)
  - May project to 2005-2006, but work has not commenced on projections

EI Task Details -cont

- EM-7
  - Develop on-road link-based emissions for HGB & BPA for each episode
  - Much of this task will be conducted by TTI with support from HGAC & TxDOT.
  - TTI Work Order has been forwarded for signatures, and will likely take 4-6 months for delivery.
  - Existing 2007 inventories have been scaled to 2005/2006 for initial CAMx runs for HGB, BPA, and rest of State
  - May 20-June 5, 2005 episode spans school and non-school days and Memorial Day holiday

EI Task Details -cont

- EM-8
  - Develop on-road non-link-based emissions for the remainder of Texas, and other states
  - Completed development of 2005 on-road mobile EI outside of Texas using NMIM instead of the 2002 NEI

EI Task Details -cont

- EM-9
  - Execute the NMIM for NONROAD emissions projections for 2005 & 2006
  - Completed for years 2005, 2006 with NMIM for states outside of Texas
  - Completed 2005, 2006 with EGAS for ships, locomotives, and aircraft for Texas and Region

EI Task Details -cont

- EM-10
  - Using the TCEQ 2002 Area, Aircraft & Locomotive Emissions Inventories for Texas, forecast as appropriate to the 2005 & 2006 episodes
  - The 2002 NEI will be used to develop forecasted emissions for these sources outside of Texas
  - Completed
  - Bonus: distributed ocean-going ships to shipping lanes in the Gulf of Mexico and the Atlantic

EI Task Details -cont

- EM-11
  - Using the new land cover for Southeast Texas, as well as episode specific temperature and satellite-based solar radiation data, develop biogenic emissions
  - We have obtained the new land cover for eastern Texas from CSR, and are processing it for GloBEIS input
  - EPA default BELD 3.1 land cover data will be used for most areas outside of Texas
  - Temperatures for 2005-2006 episodes have been kriged
  - Satellite-derived solar data have been downloaded, and we are processing it for GloBEIS input now

EI Task Details -cont

- EM-12
  - Incorporate updated emissions provided by various regulated entities (e.g., marine shipping, aircraft)
  - No updates yet
  - None may come forward with new data

EI Task Details -cont

- EM-13
  - Update EPS3 and associated software to process chemical species for CB05
  - Will process with CB-IV first, then try CB05

EI Task Details -cont

- EM-14
  - Select point sources for the Plume-in-Grid algorithm, for treating elevated plumes more realistically
  - Likely use a somewhat modified procedure from previous modeling, and will run a few tests in EPS3, then in CAMx
  - EPS3 processing of all the elevated points must come first; still several weeks away

EI Task Details -cont

- EM-15
  - Execute EPS3 to create gridded and hourly-speciated, episode-specific CAMx-ready elevated and low-level emissions
  - Complete for area and non-road
  - Mobile source back-projected 2007 to 2005 ready for preliminary CAMx runs
  - Point Source 2004 ready for preliminary runs with hourly 2005 updates

EI Task Details -cont

- EM-16
  - Evaluate the speciated emissions comparing them with results from data analysis
  - Not doing this for preliminary modeling
  - Need to develop a speciated EI first
  - Need to have some TexAQS II and Auto-GC data analyzed first

Staff by EI Category

- **Point Sources**
  - Ron Thomas
  - Marvin Jones
  - Barry Exum, Jocelyn Mellberg
- **Area & Non-road Mobile**
  - Jim MacKay
- **On-road Mobile**
  - Chris Kite
- **Biogenics**
  - Mark Estes
  - Clint Harper

Questions