TEXAS COMMISSION ON ENVIRONMENTAL QUALITY

# Preparing Point Source Emissions Inventories For Ozone SIP Modeling

## Base Case and Future Case

45 Pages
April 26, 2005

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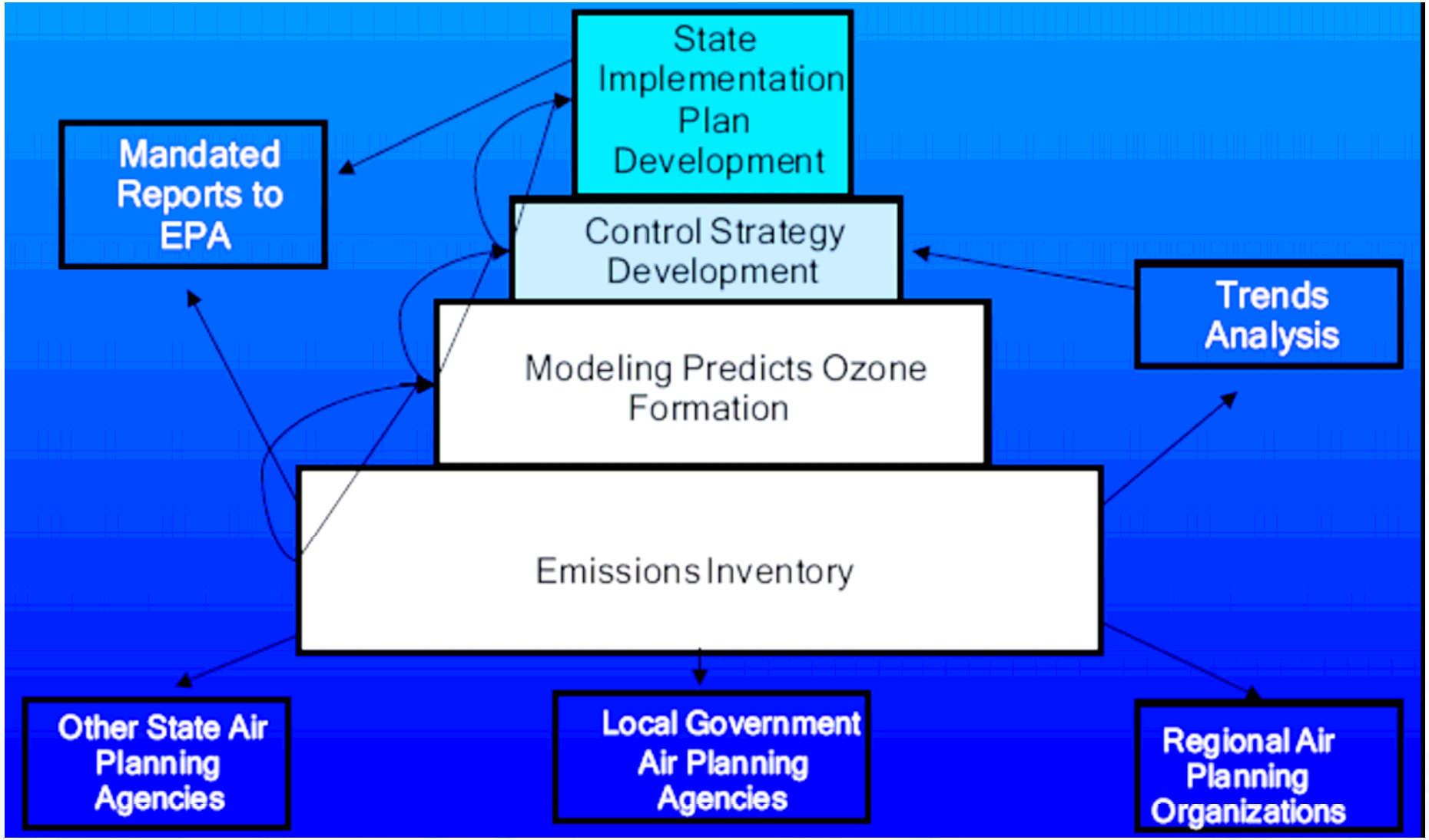
Air Quality Planning and Implementation Division

# Emissions Inventory Modeling

- **Point Sources**
  - Ron Thomas, Jocelyn Mellberg
- Area & Nonroad Sources
  - Jim MacKay
- Onroad Mobile Sources
  - Chris Kite
- Biogenic Sources
  - Mark Estes

# EI – Use in Planning



# HGB 8-co Emissions Summary

| Emission Category | NOx August 30 (tons/day) | | VOC August 30 (tons/day) | |
|---|---|---|---|---|
| | 2000 | 2007 | 2000 | 2007 |
| Point | 492 | 163 | 384 | 245 |
| Area/Nonroad | 184 | 156 | 254 | 234 |
| Mobile | 342 | 175 | 151 | 89 |
| Bio* | 19 | 19 | 1251 | 1251 |
| Total | 1037 | 513 | 2040 | 1819 |

* August 25

# SIP & Modeling Web Sites

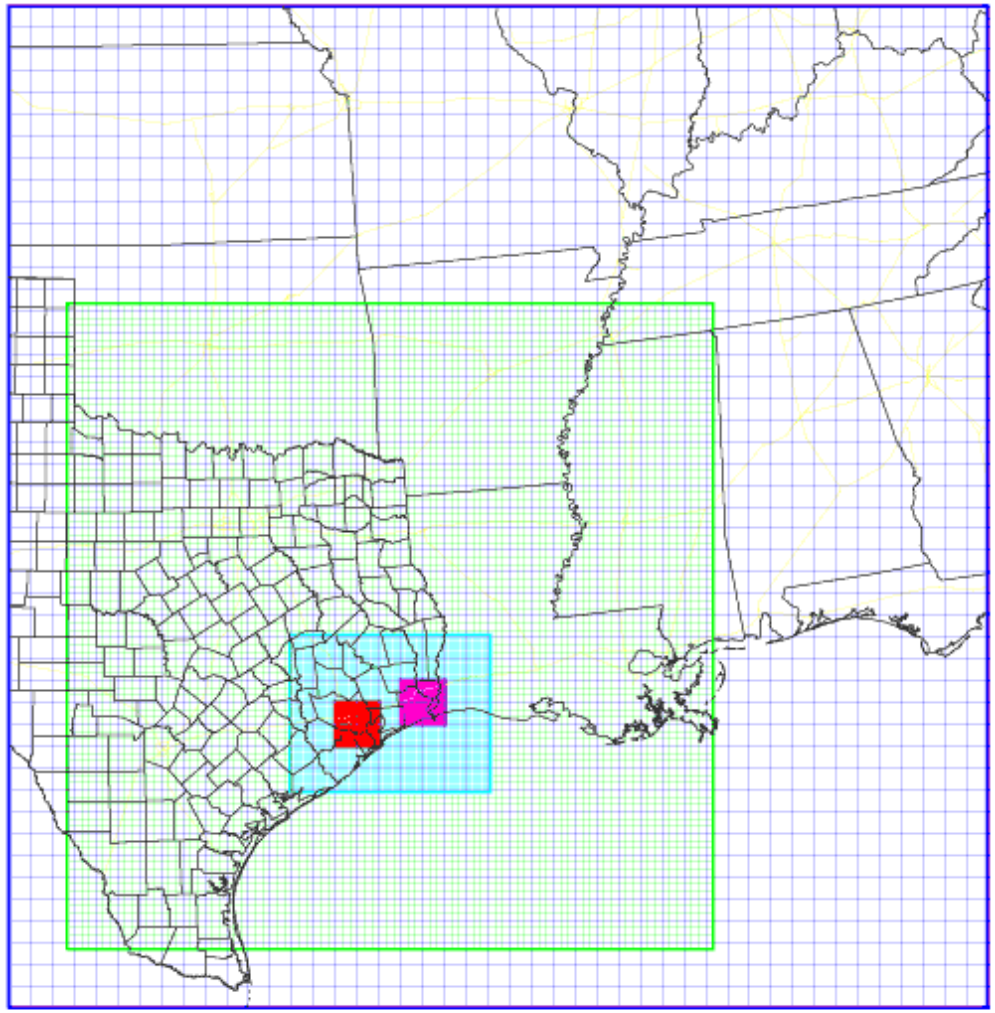
http://www.tnrcc.state.tx.us/oprd/sips/

http://www.tnrcc.state.tx.us/oprd/sips/siphga.html#Current

http://www.tnrcc.state.tx.us/oprd/sips/june2004hgb_EDrec.html

Internal http://amda

# Modeling Domain



Regional East Texas HGBPA HG BPA

# SIP Model Input Requirements

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

# Point Sources

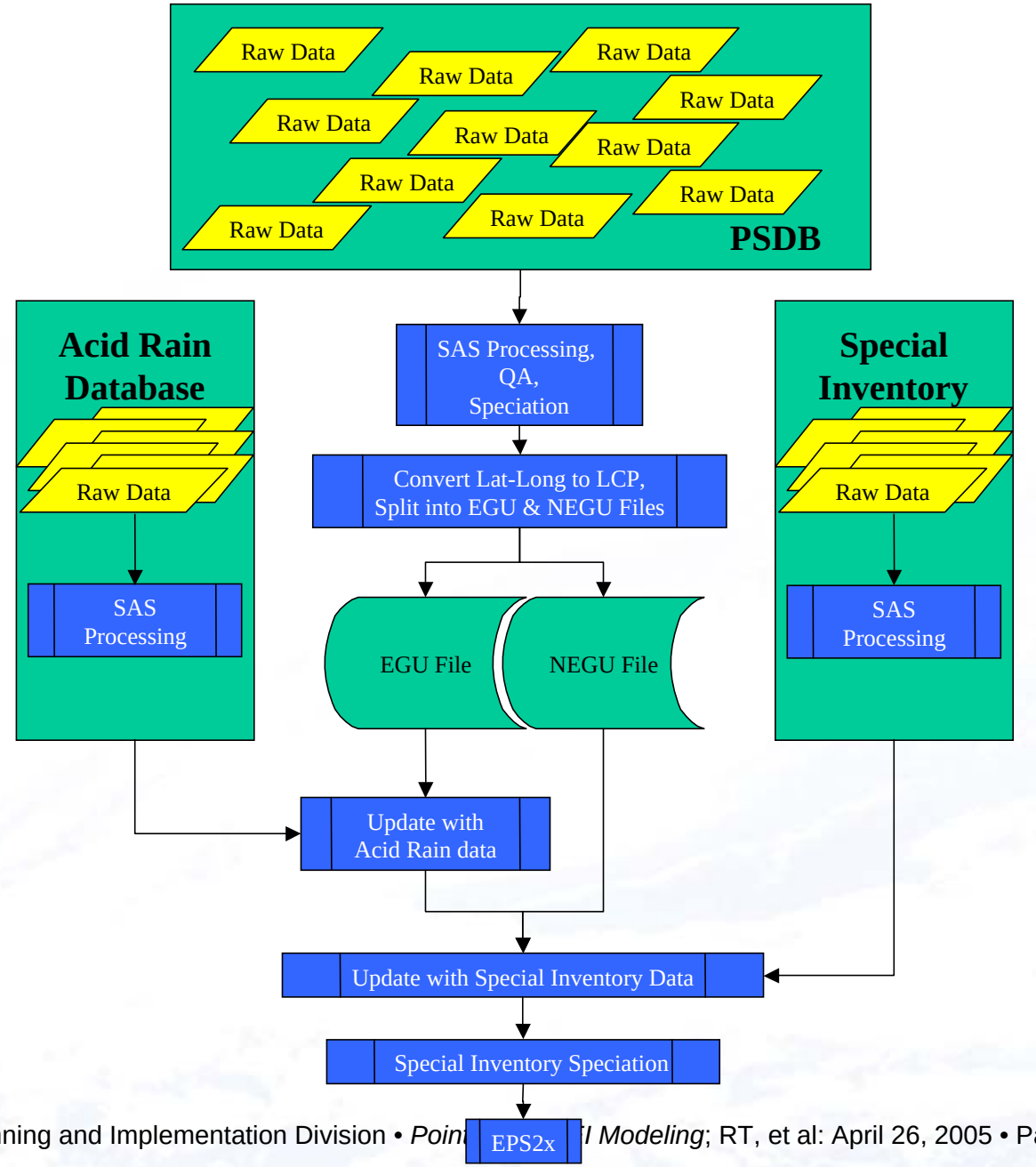
# Sources of Modeled Data (Base Case)

- PSDB/STARS snapshot (IEAS,Modelers)
- Special Inventory (IEAS,Modelers)
- Upset/Maintenance Database (Regional Office,Modelers)
- Acid Rain Program CEM (EPA,Modelers)
- Louisiana (LDEQ)
- Offshore (MMS)
- Regional (NEI)
- Mexico (BRAVO)

# Domain-Wide Point Source Summary for August 30, 2000

| | $NO_X$ (tpd) | VOC (tpd) | CB-IV HC (tpd) |
|---|---|---|---|
| **TEXAS EGU** | 1348.26 | 19.63 | 19.24 |
| **TEXAS NEGU** | 866.39 | 500.67 | 458.37 |
| **REGION 12 U/M** | 0.00 | 3.01 | 3.32 |
| **HGB OLEFIN ADJUSTMENT** | 0.00 | 155.36 | 177.84 |
| **LOUISIANA EGU** | 404.04 | 3.29 | 3.31 |
| **LOUISIANA NEGU** | 630.90 | 218.79 | 197.25 |
| **OTHER EGU** | 5739.74 | 39.28 | 43.20 |
| **OTHER NEGU** | 2017.41 | 1769.35 | 1569.15 |
| **OFFSHORE POINTS** | 546.08 | 188.85 | 56.03 |
| **MEXICO POINTS** | 272.34 | 0.41 | 0.31 |
| **TOTALS** | 11825.16 | 2898.64 | 2528.02 |

# Processing Texas Point Sources



# Create AFS Records

- AIRS Facility Subsystem (AFS)
- One record for each Account/FIN/EPN/SCC/Pollutant combination
- Pollutant
  - NOx
  - VOC
  - CO
- Emission Rate
  - Annual
  - Ozone-Season Daily
  - Hourly

# AFS Records

- Example Record

```
B 00 00 AC 48157 HG    4911   10100222 0005 0018
  014    PO 00081800 00090700   423.3336 -1139.5708
  152.4 6.707   416  25.3  21  26  28  25 24  0 7
  8736 42603   23.64131
  FG0020V 8          WAP8                    P
  RELIANT ENERGY INC                  FORT BEND
  ARCOLA          NOx                          D
  ST 08/27/2001 PSDB
```

# Modeling Inventory QA

- Non-VOCs
- Top 100 NOx & VOC check with IEAS
- Geographic Location
- Stack Parameters
- Ozone-Season Daily calculation

# Rule Effectiveness (RE)

- Estimate of actual in-use control efficiency, over time
- EPA requires RE to be applied to VOC emission rates for NEI reporting and ozone modeling
  - Applied only to controlled sources via TCEQ SAS program
- Reason that modeling inventory (AFS file) does not always match reported EI (PSDB/STARS)
  - Increases overall VOCs by about 25%
- Criteria and factors currently being reviewed by EPA to include compliance, maintenance, inspections, other pollutants, etc.

# EPS

- Emissions Preprocessing System
- Improved Periodically by Contractor
- Assists with Allocation of Emissions
  - Spatially
    - Assign low-level emissions to specific grid cells
    - Elevated emissions maintains 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, SAPRC)

# Spatial Allocation

- Low-level (plume rise < 30m)
  - Lumped into grid cells
  - Smaller grid cells (higher resolution) closer to HGA
  - Added to all other parts of gridded EI at final EPS merge step
- Elevated
  - Modeled initially from point of reported coordinates
  - Modeled initially from calculated plume rise height in CAMx
- QA
  - Tileplots

# Temporal Allocation

- AFS 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 record
  - Many AFS records will share same profile
- QA
  - Tileplots

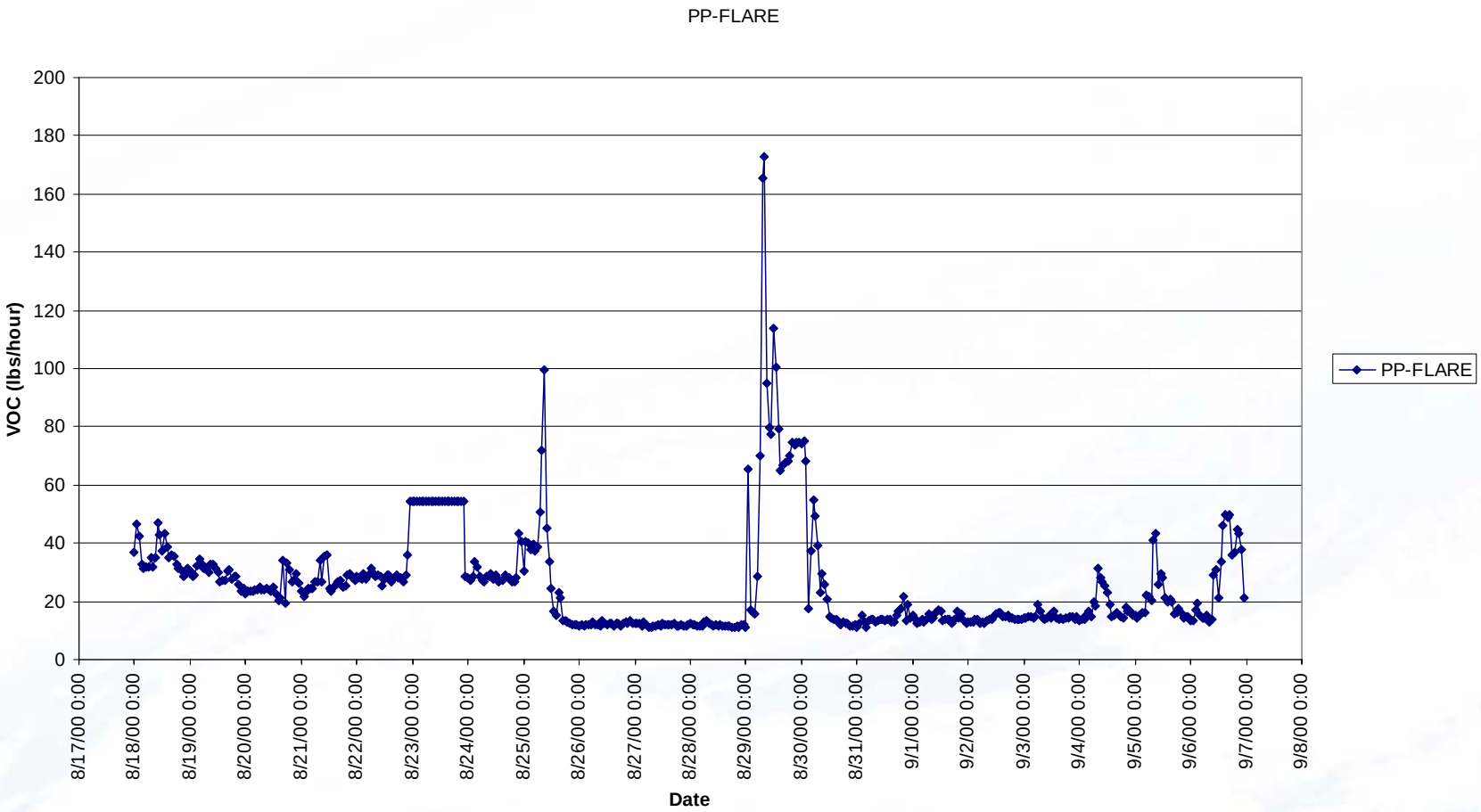
# Temporal Allocation

- Hour Specific Data
  - Do not receive Temporal adjustment/profile
  - Provide for true bottom-up hourly modeled emissions
  - EPA Acid Rain Program CEM
    - Hourly data received, housed and QA'd by EPA
    - TCEQ creates xref between Acid Rain Program boiler identifiers and PSDB/NEI identifiers
    - First in nation to use these data for SIP purposes
  - Special Inventory
    - TexAQS 2000
  - Region 12 Upset/Maintenance

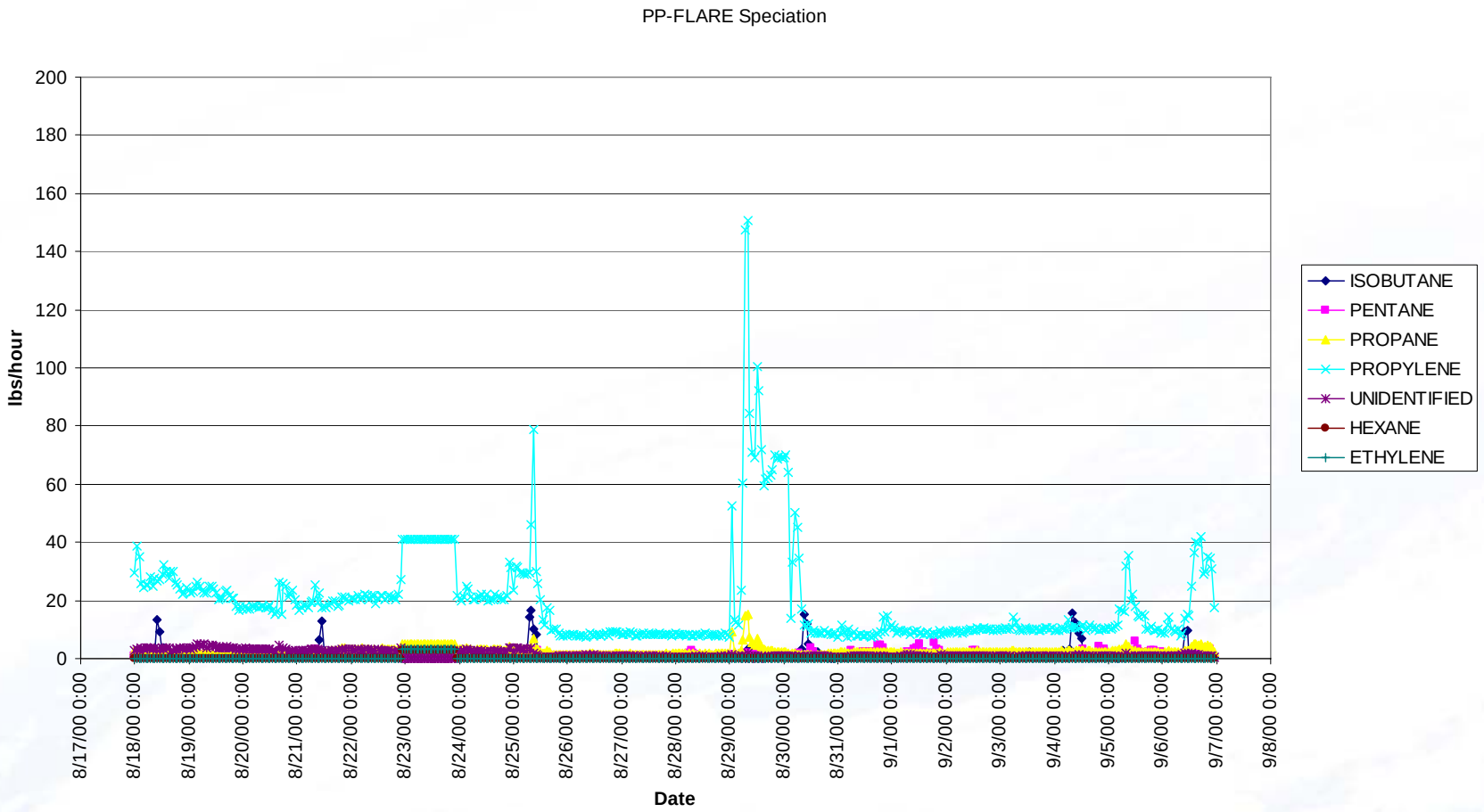
# Special Inventory

- 83 Top NOx and VOC emitters in HGA and BPA were asked to report hourly emissions that varied by more than 20% of normal operations

# Special Inventory Data



# Special Inventory Data



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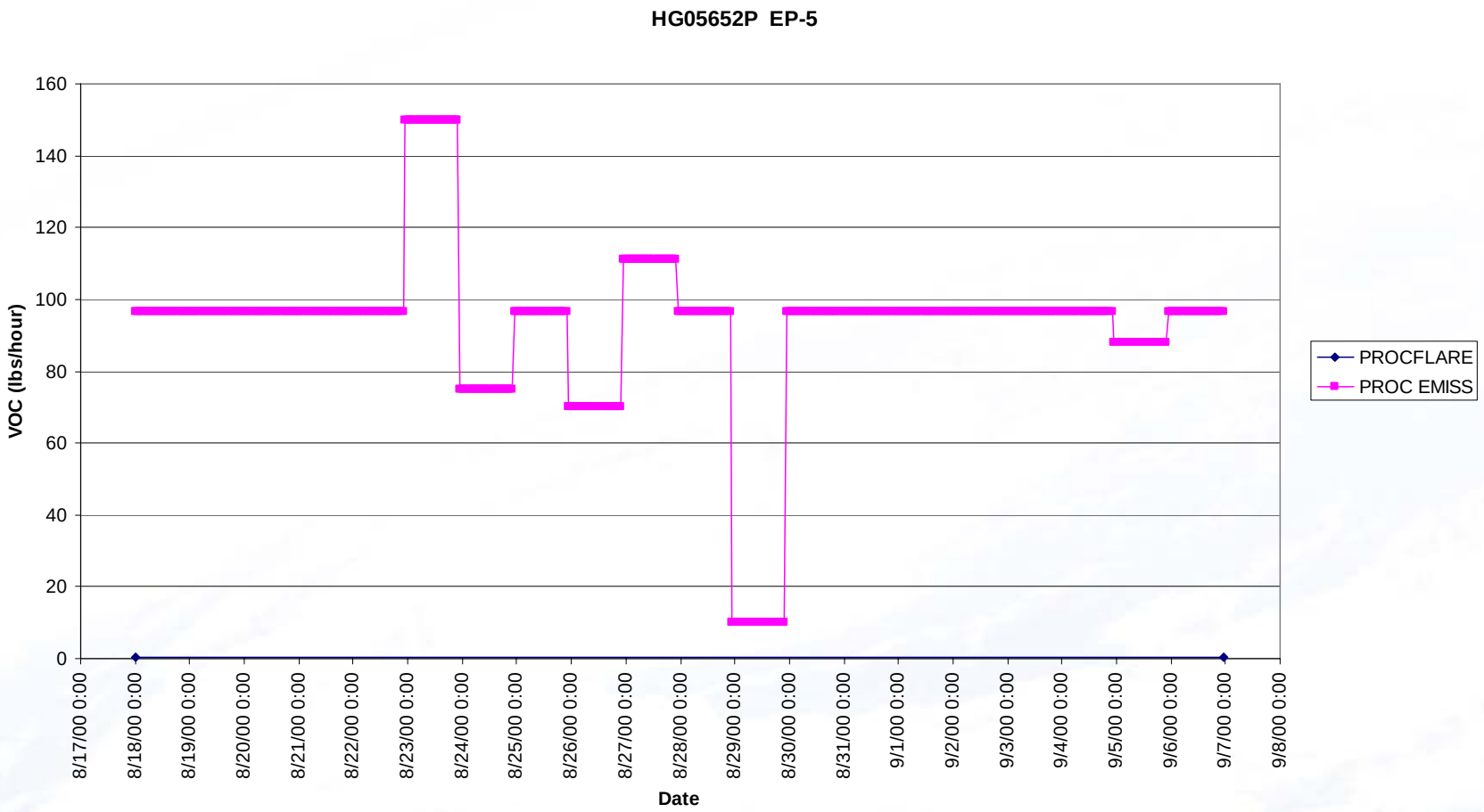
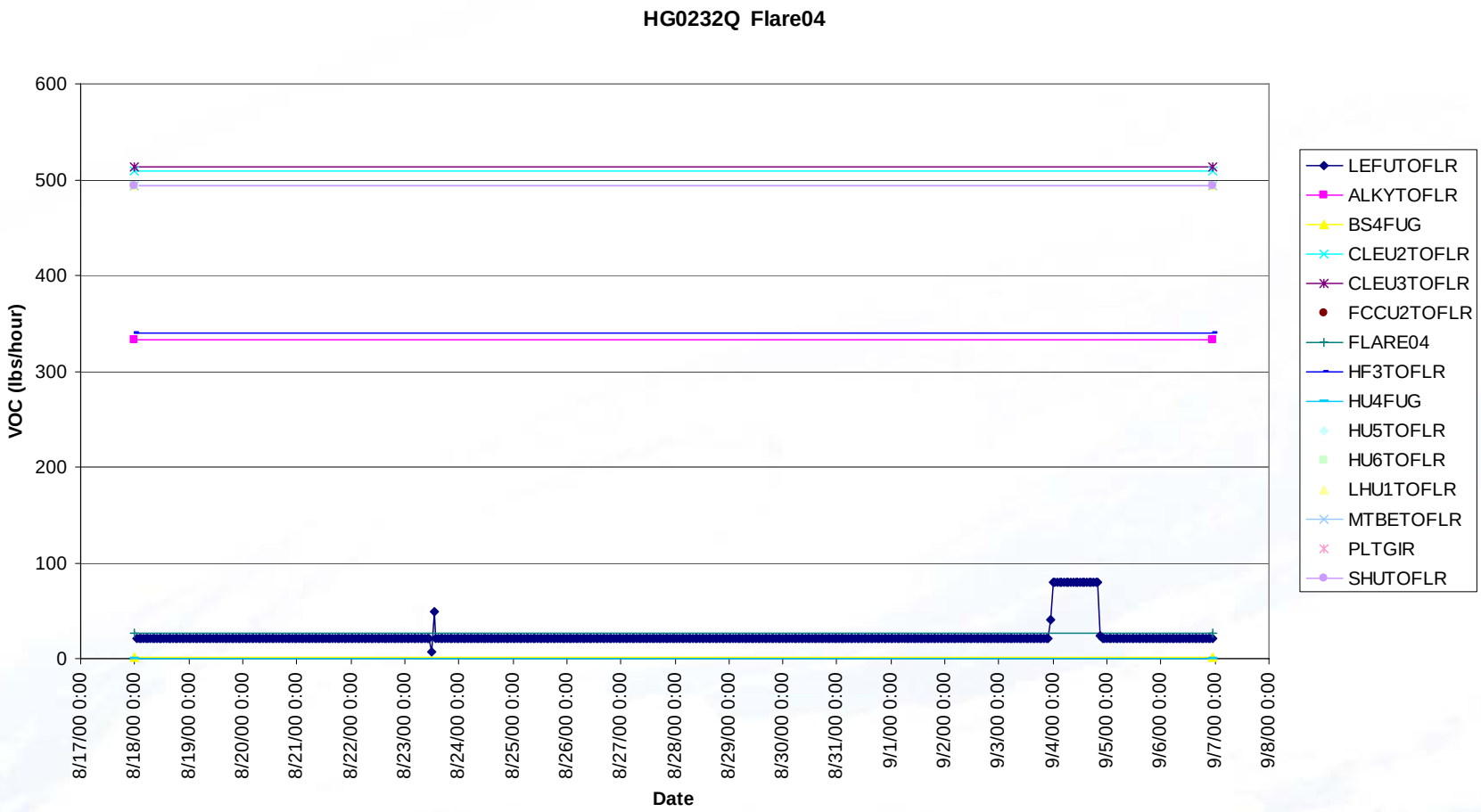


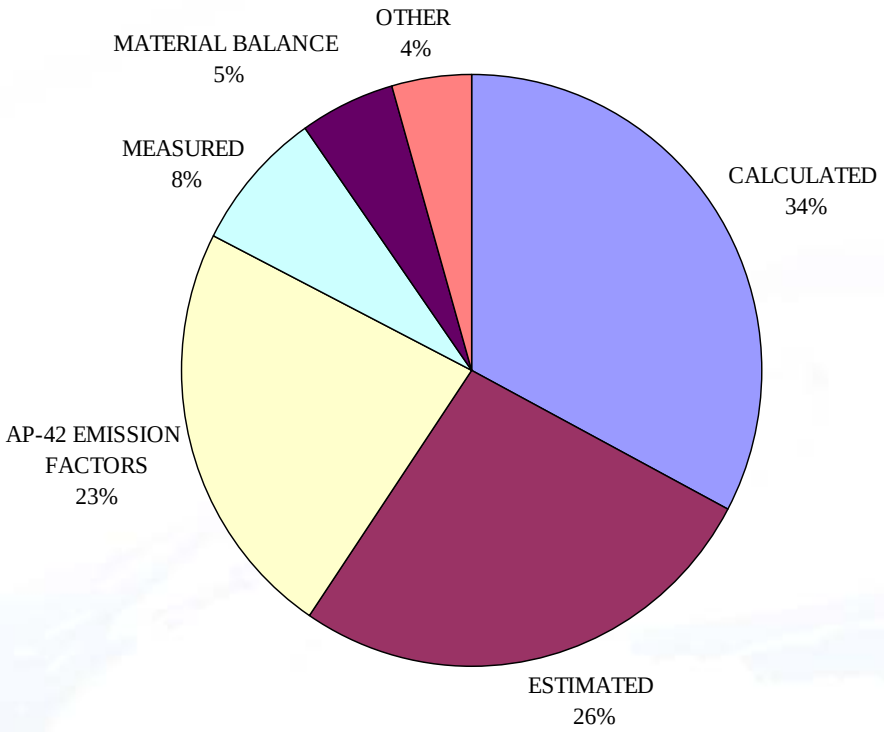
# Special Inventory Data



# Region 12 Upset/Maintenance

- Examined emission events reported during modeling episode
- Limited Data
  - Some Speciation Data
  - Try to match emission point
- Cross reference with Special Inventory
- Include events not already reported to Special Inventory

# 2000 HG VOC Emissions by EI Method




**Calculated**
Calculated from engineering principles

**Estimated**
Estimated from production data

**AP-42 Emission Factors**
Calculated from EPA emission factors or tank calulations based upon them

**Measured**
Based upon a single stack test

**Material Balance**
Calculated from material handled, e.g. paint applied

**Continuous Monitoring**
Measured by a continuous stack monitor

Dataset: Oracle.psdb_alloc_2000_v15

Tileplot

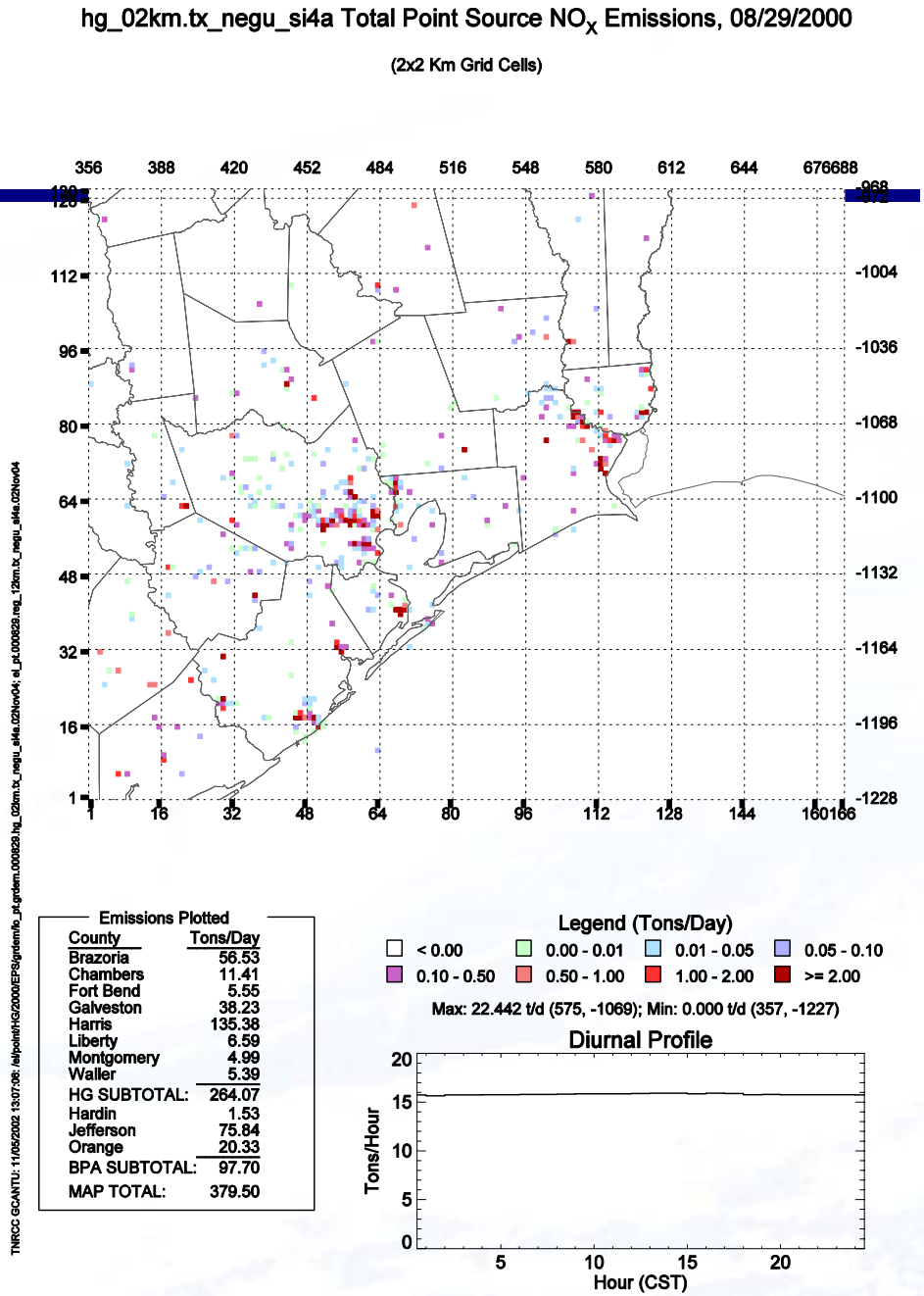
SE Texas

2 km grid

NEGU w/ SI

NOx

8/29/2000



Tileplot

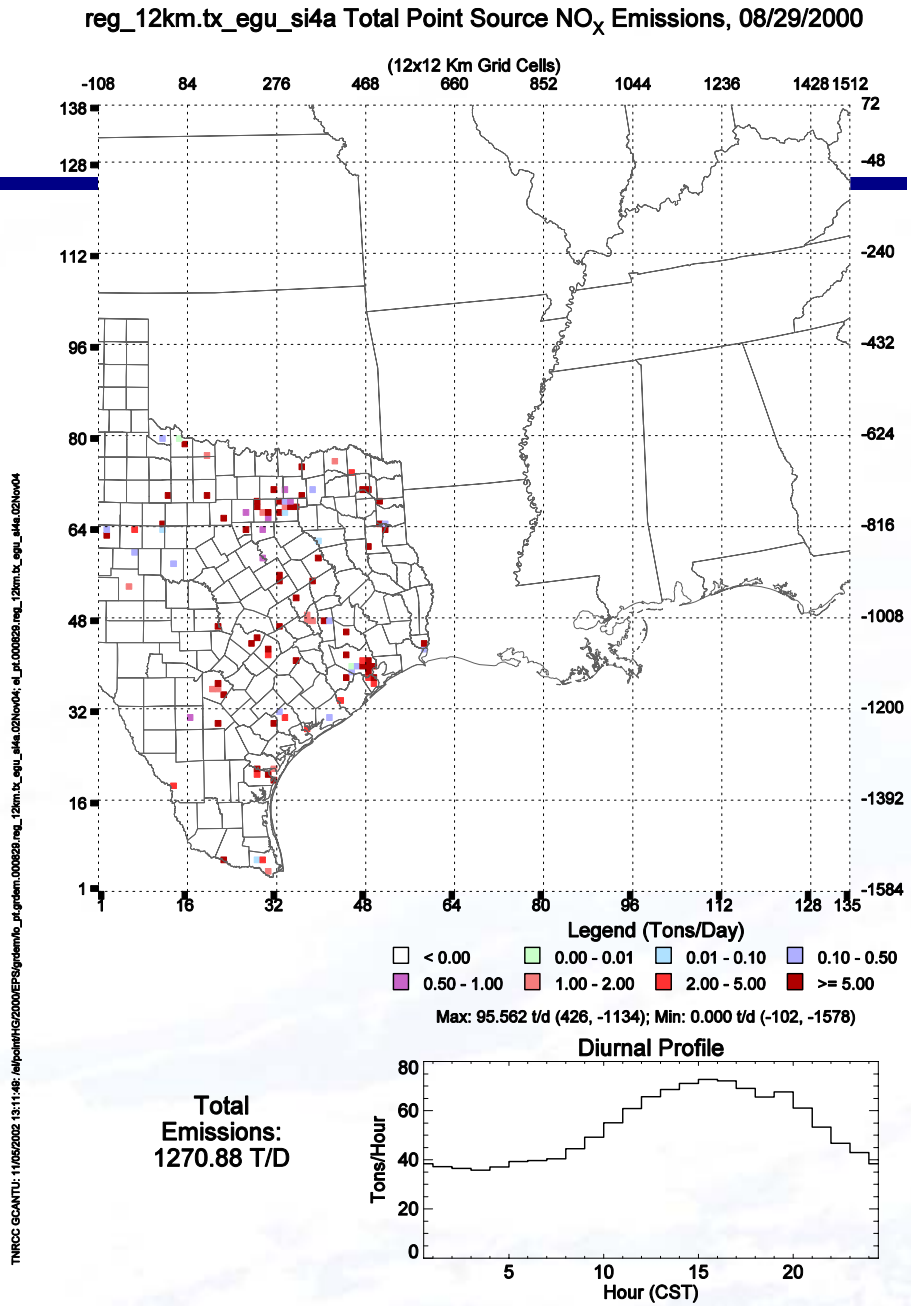
Texas

12 km grid

EGU w/ SI

NOx

8/29/2000



Tileplot

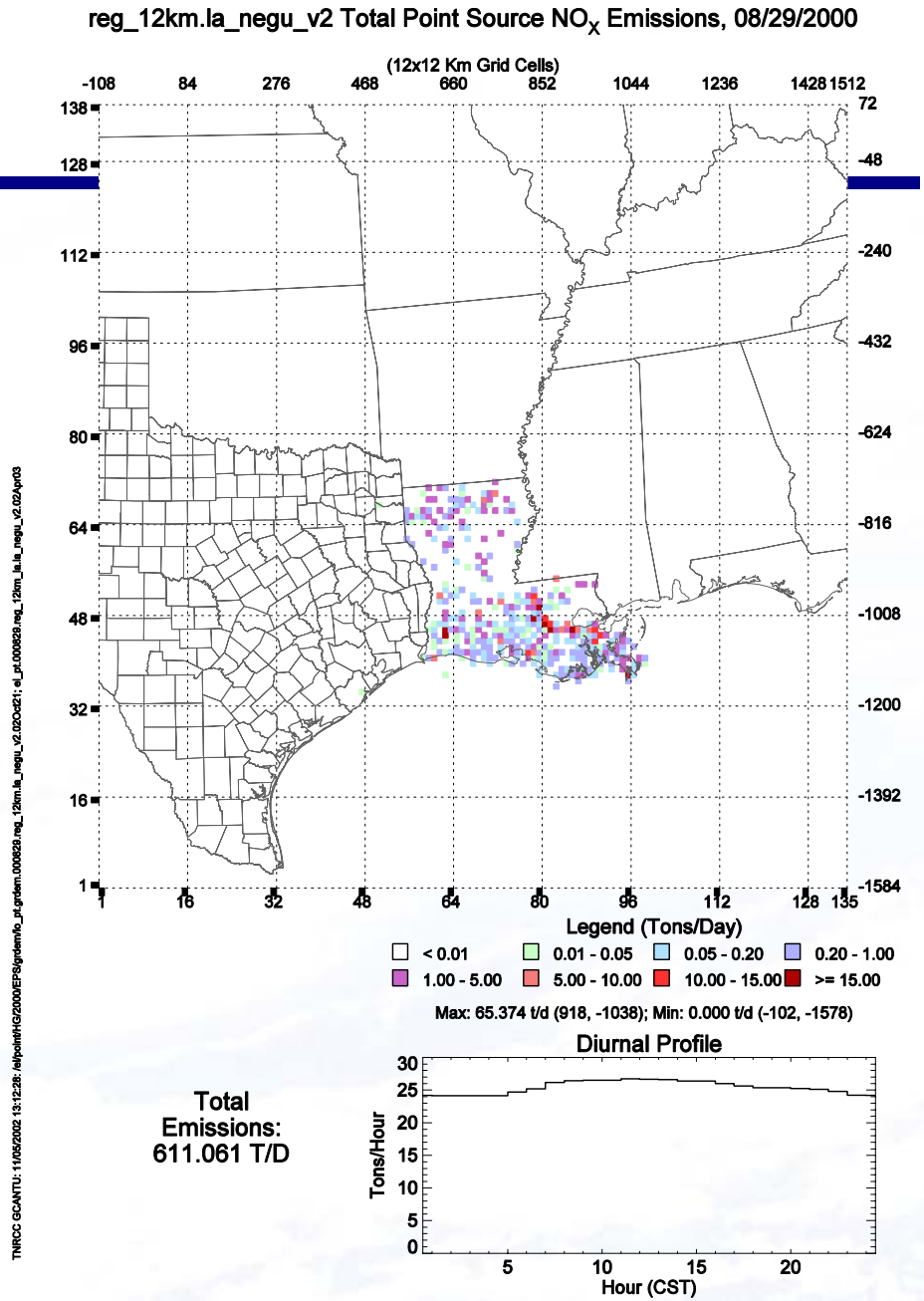
Louisiana

12 km grid

NEGU

NOx

8/29/2000



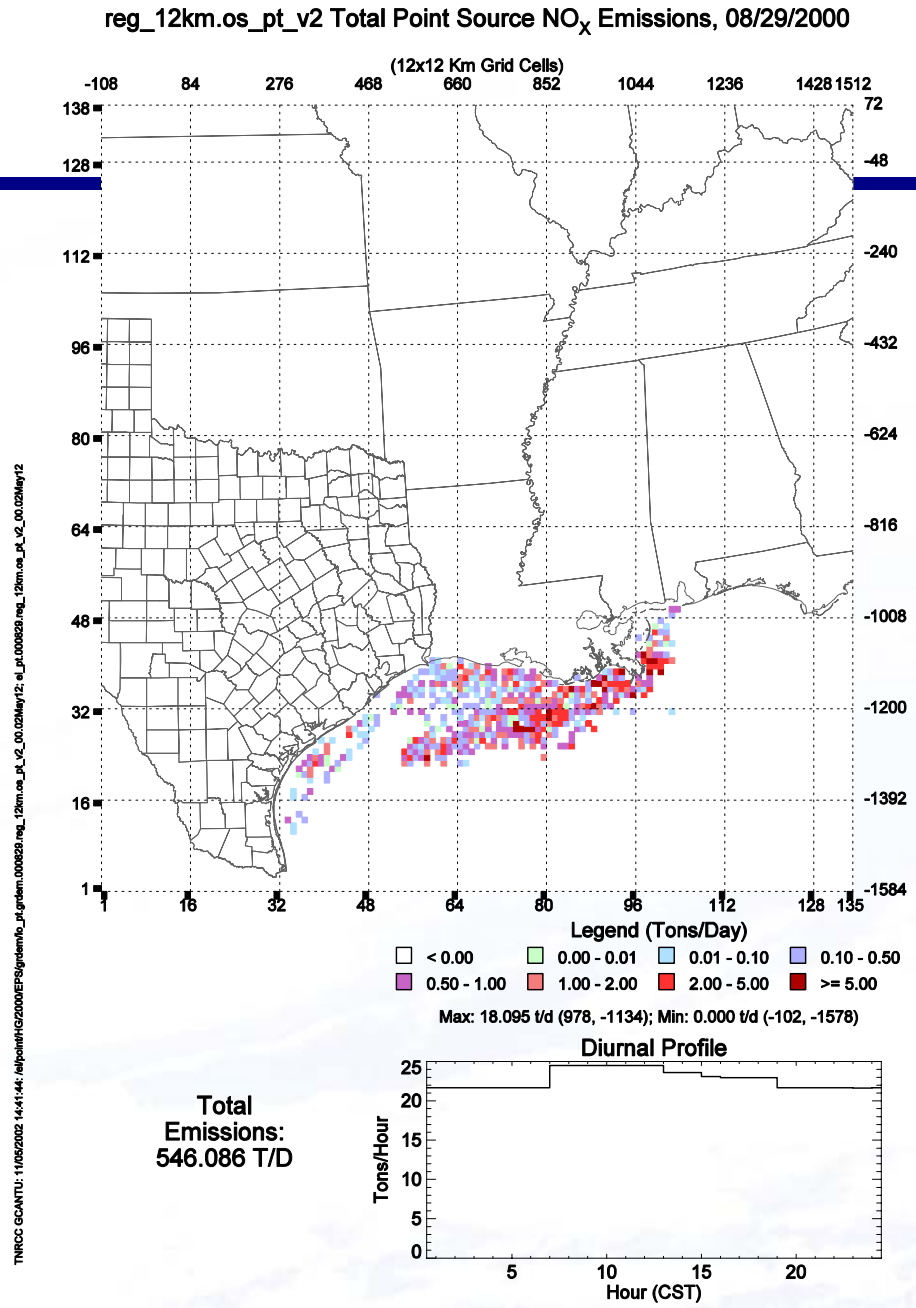
Tileplot

Offshore

12 km grid

NOx

8/29/2000



Tileplot

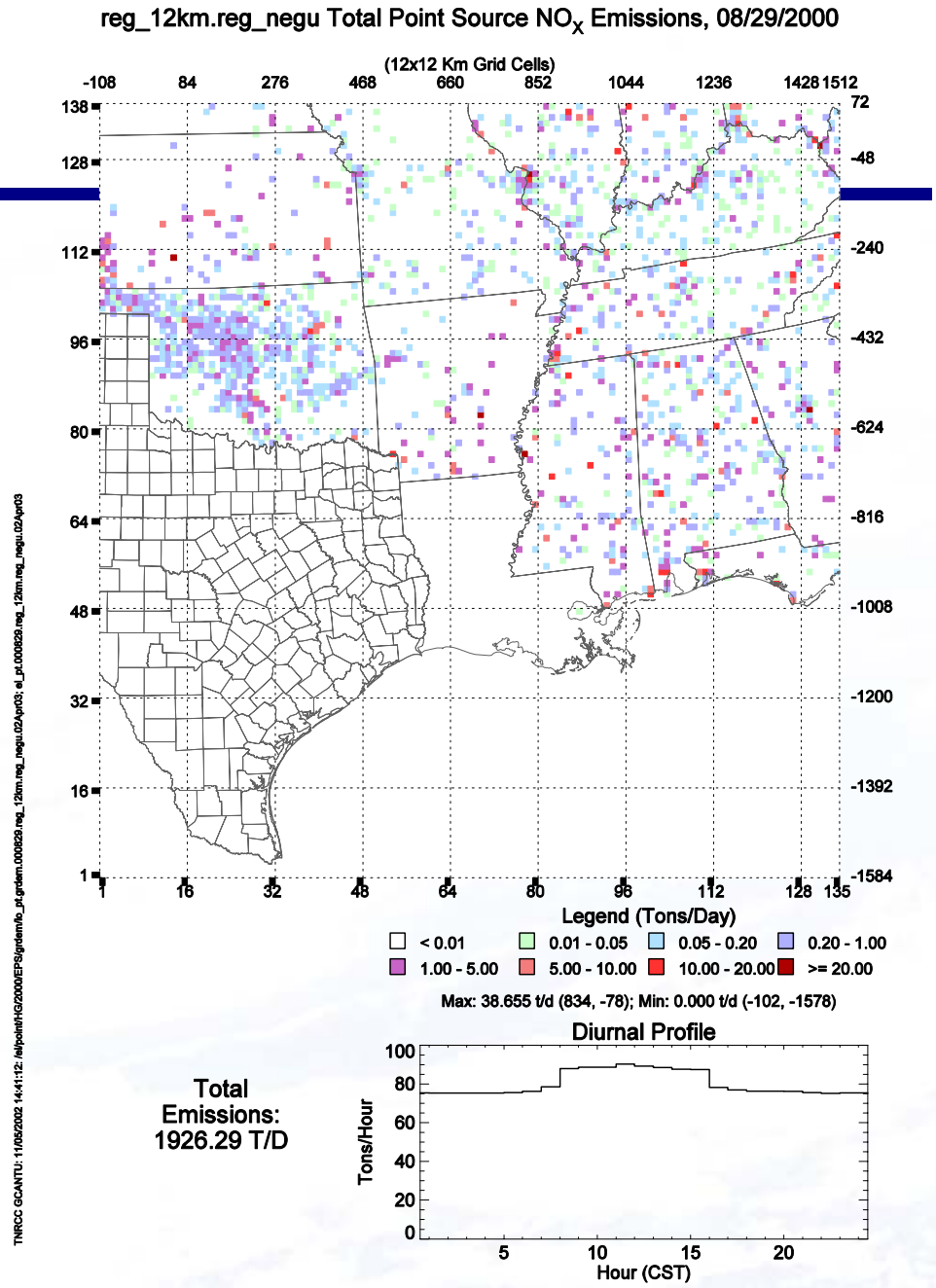
Region

12 km grid

NEGU

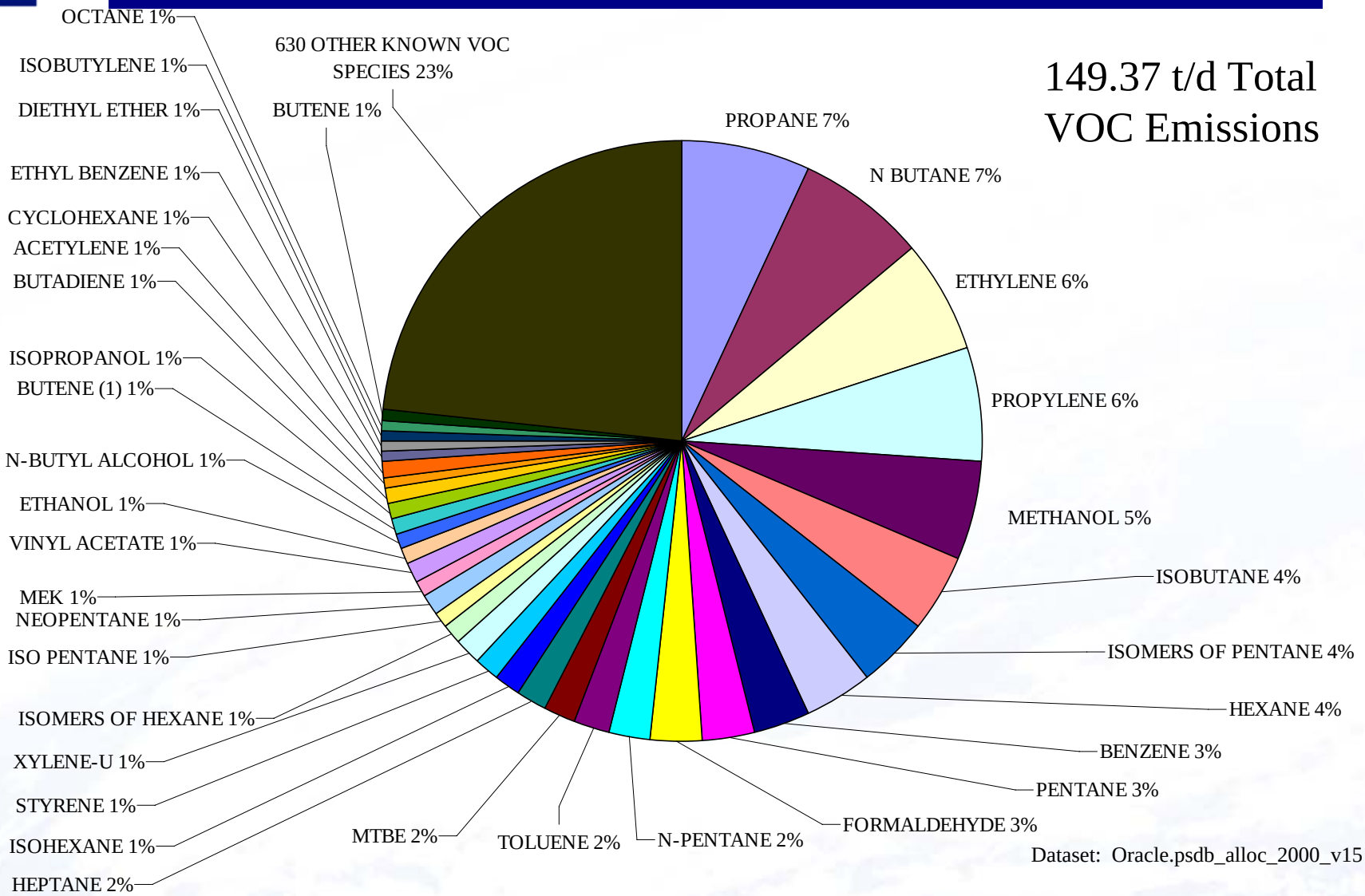
NOx

8/29/2000



# Estimated 2000 HG 8 County VOC Speciation

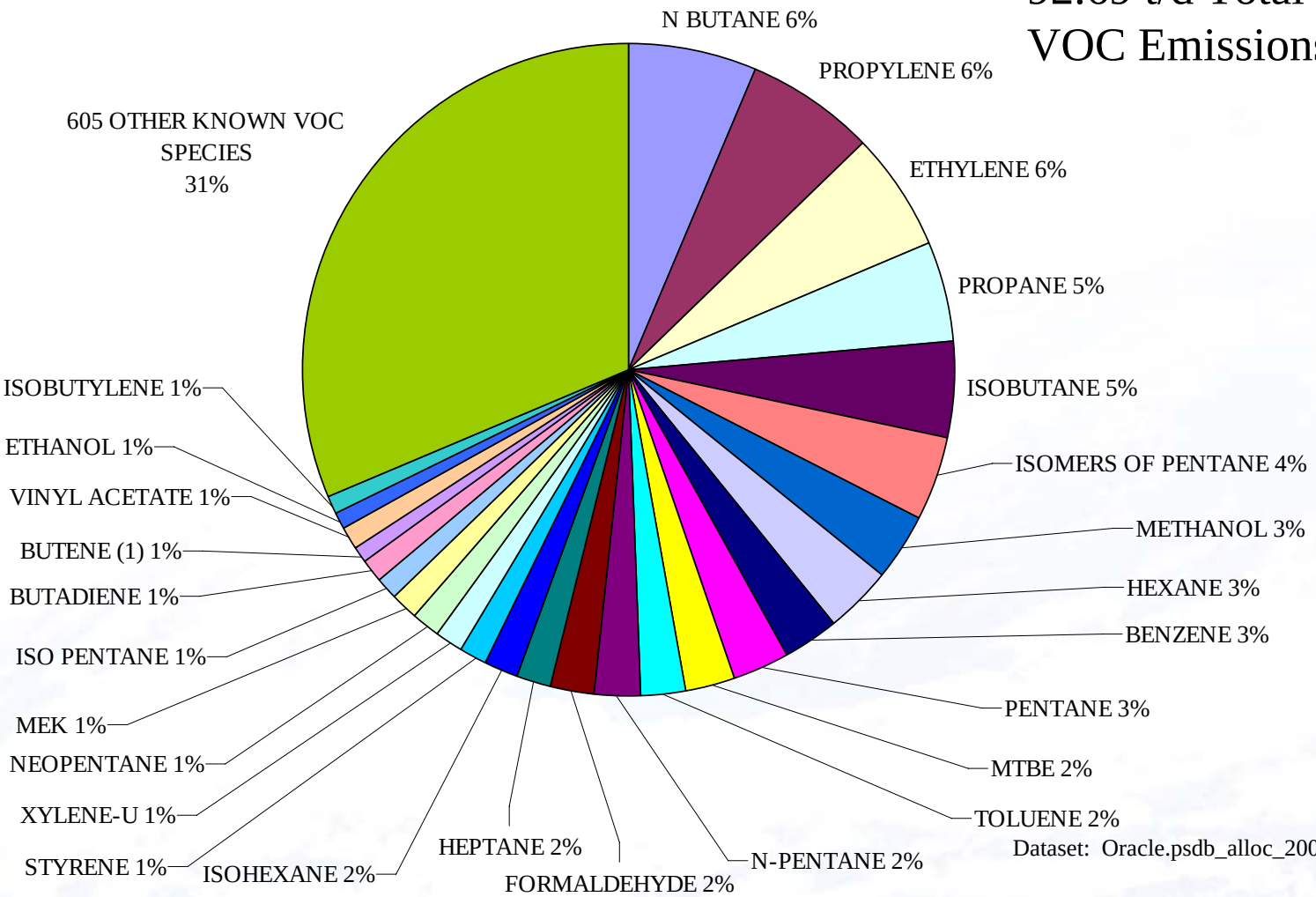
149.37 t/d Total VOC Emissions




Dataset: Oracle.psdb_alloc_2000_v15

# Estimated 2000 Harris County VOC Speciation

92.69 t/d Total VOC Emissions




Dataset: Oracle.psdb_alloc_2000_v15

# Point Source Speciation

- Historically
  - Used standard, EPA-default profiles and xrefs
  - Specific contracts to update specific categories
- Dec. 2002 SIP
  - Improved speciation of reported EI (IEAS Guidance)
  - PES/Environ contracts to generate emissions profiles
  - If a source was 75% + speciated, use that speciation for all of that source's emissions
  - Otherwise, use Texas SCC-average or EPA default speciation
- June 2004 SIP
  - Use compound-specific emissions as reported for all sources
  - For unspeciated portion, apply default profile, after removing non-VOC and common species from the profiles)

# Current Speciation Method

- PSDB
  - Remove non-VOC compounds
  - Refine speciation with Crude Oil, Gasoline, Naphtha, Stoddard Solvent, and Refinery profiles
  - Examine Unspeciated VOC mixtures and set to NONMETHANE VOC-U, CONTAM 50001
- EPA Default Profiles
  - Delete non-VOC/non-Reactives
  - Normalize
  - Check for profiles composed of only one compound
    - Replace with appropriate profile (SPECIATE, CARB)
- "Speciation of Texas Point Source VOC Emissions for Ambient Air Quality Modeling", G. Cantu, July 2003
  - ftp://ftp.tnrcc.state.tx.us/pub/OEPAA/TAD/Modeling/HGAQSE/Modeling/EI/PointEI_VOC_Speciation_Report-GabrielCantu.pdf

# Sample Speciation Process

**Sample Point**

Account: XY3456Z

FIN: A-1

EPN: B234

SCC: 12345678

**Reported Species**

| | |
|---|---|
| Nonmethane VOC-U | 80.0 % |
| Pentane | 10.0 % |
| Propane | 4.0 % |
| N-Butane | 2.0 % |
| Benzene | 2.0 % |
| Ethylbenzene | 2.0 % |

**Intermediate A-1/B234/9876 Profile**

| | |
|---|---|
| Isomers of Hexane | 25.0 % |
| Isomers of Heptane | 31.4 % |
| Isomers of Octane | 25.0 % |
| C7 Cycloparaffins | 5.0 % |
| C8 Cycloparaffins | 1.5 % |
| Isomers of Pentane | 11.0 % |
| Isobutane | 1.1 % |

**SCC Profile Assignment: 9876**

| | |
|---|---|
| Isomers of Hexane | 5.0 % |
| Isomers of Heptane | 6.0 % |
| Isomers of Octane | 5.0 % |
| C7 Cycloparaffins | 1.0 % |
| C8 Cycloparaffins | 0.3 % |
| Isomers of Pentane | 2.1 % |
| Methane | 61.3 % |
| Ethane | 8.0 % |
| Propane | 7.0 % |
| N-Butane | 4.0 % |
| Isobutane | 0.2 % |
| Benzene | 0.1 % |

**Augmented Profile 9876**

| | |
|---|---|
| Isomers of Hexane | 16.0 % |
| Isomers of Heptane | 20.0 % |
| Isomers of Octane | 16.0 % |
| C7 Cycloparaffins | 3.0 % |
| C8 Cycloparaffins | 1.0 % |
| Isomers of Pentane | 7.0 % |
| Propane | 23.0 % |
| N-Butane | 13.0 % |
| Isobutane | 0.7 % |
| Benzene | 0.3 % |

**Resulting A-1/B234 Speciation**

| | | | |
|---|---|---|---|
| Isomers of Hexane | 20.0 % | Pentane | 10.0 % |
| Isomers of Heptane | 25.0 % | Propane | 4.0 % |
| Isomers of Octane | 20.0 % | N-Butane | 2.0 % |
| C7 Cycloparaffins | 4.0 % | Benzene | 2.0 % |
| C8 Cycloparaffins | 1.0 % | Ethylbenzene | 2.0 % |
| Isomers of Pentane | 9.0 % | | |
| Isobutane | 1.0 % | | |

# HRVOC Imputation

- TexAQS 2000 study results
  - Researchers agree that the reported EI under-estimates the amount of real-world industrial VOC concentrations
  - Compared to ambient measurements
    - Auto-GCs
    - Baylor aircraft flights
- See SIP documentation

# 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 |

# Sources of Modeled Data (Future Case)

- Base Case Inventory
- TIPI/EGAS Growth (Modelers)
- Banking and Trading Program (APD,Modelers)
- New EGUs
  - TCEQ Turbine List (APD Permits)
  - PUC Project List for Proposed and Cancelled
  - Permit Retrieval & Data Matching/Formatting (Modelers)
- TCEQ Rules
  - Chs. 115, 117, 101 (Policy,Modelers)
  - MECT (Mass Emissions Cap & Trade) = NOx Cap
  - HECT (HRVOC Emissions Cap & Trade) = HRVOC Cap
- $NO_X$ Sip Call (Modelers)
- Louisiana SIP (Modelers)

# TIPI

- Texas Industrial Production Index
- Value Added Index
  - Based on weighted average of employment, man hours, and production data
  - Underlying process to derive data same as BEA gross-state product
  - http://www.dallasfed.org/data/data/mi5000.tab.htm
- Data is more recent than EGAS 4.0
  - EGAS
    - 1996 Baseline
    - Last updated Jan. 2001
  - TIPI
    - Jan. 1967 - Nov. 2003 Linear Regression

# Future Case (2007) Non-TX Growth & Controls

- Growth
  - Regional Points
    - EGAS
  - Louisiana Points
    - EGAS
  - Offshore
    - None
  - Mexico
    - None
- Controls
  - Regional Points
    - $NO_X$ Sip Call (February 2, 2002 Federal Register)
  - Louisiana Points
    - Baton Rouge 9-Parish $NO_X$ (12/2001) SIP
  - Offshore
    - None
  - Mexico
    - None

# Future Case (2007) HGB Growth & Controls

- Growth
  - EGU
    - New EGUs
    - 0.0 tpd $NO_X$
    - 0.0 tpd VOC
  - NEGU
    - Banked $NO_X$ & VOC
    - 0.0 tpd $NO_X$
    - 13.2 tpd VOC
- Controls
  - EGU
    - 2007 $NO_X$ Cap
  - NEGU
    - 2007 $NO_X$ Cap
    - HRVOC Cap

# Future Case (2007)
# HGB Growth & Controls

**Table 3-29: HGB 8-County Ozone Season Daily (OSD) NOx Cap Summary**

| **HGB sources** | **2000 NOx OSD (tpd)** | **2000 NOx w/Acid Rain (tpd)[1]** | **2007 MECT NOx Cap (tpd)** | **2008 MECT NOx Cap (tpd)** | **2007 Modeled NOx (tpd)2** |
|---|---|---|---|---|---|
| EGU | 192 | 203 | 23 | 23 | 25 |
| NEGU | 283 | 283 | 113 | 104 | 135 |
| **Total** | 475 | 486 | 136 | 127 | 160 |

[1] average day of the hourly Acid Rain data over 20-day episode
[2] includes all 4 of the summed estimates above; excludes non-MECT bank
NOTE: gridded vs. non-gridded emissions summaries may vary slightly

# Future Case (2007) ETX Growth & Controls

- Growth
  - EGU
    - New EGUs
    - 70.7 tpd $NO_X$
    - 13.6 tpd VOC
  - NEGU
    - Newly Permitted Units/Modifications to Cement Kilns
    - TIPI/EGAS
- Controls
  - EGU
    - SB7 $NO_X$ controls
    - Ch. 117 $NO_X$ Controls
  - NEGU
    - Agreed Orders and Consent Decree