Estimates of Secondary Organic Aerosol Formation in Houston, Texas

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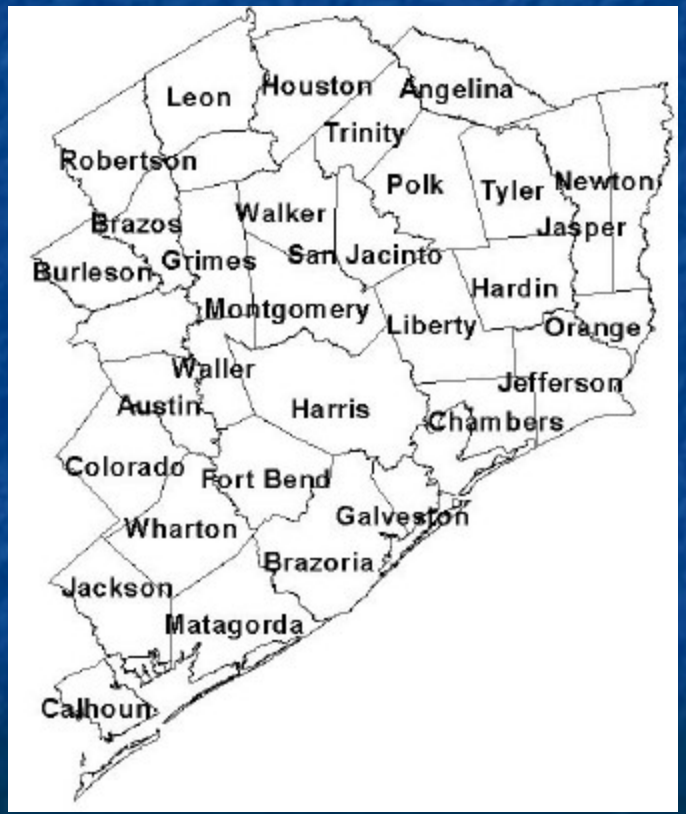
SOA formation 1: Inventory Analysis

- Anthropogenic emissions and speciation data gathered for SouthEast Texas
- Fractional Aerosol Coefficients (FAC) were applied as a first approximation of Secondary Organic Aerosol (SOA) from individual VOC compounds



Emissions/FAC data

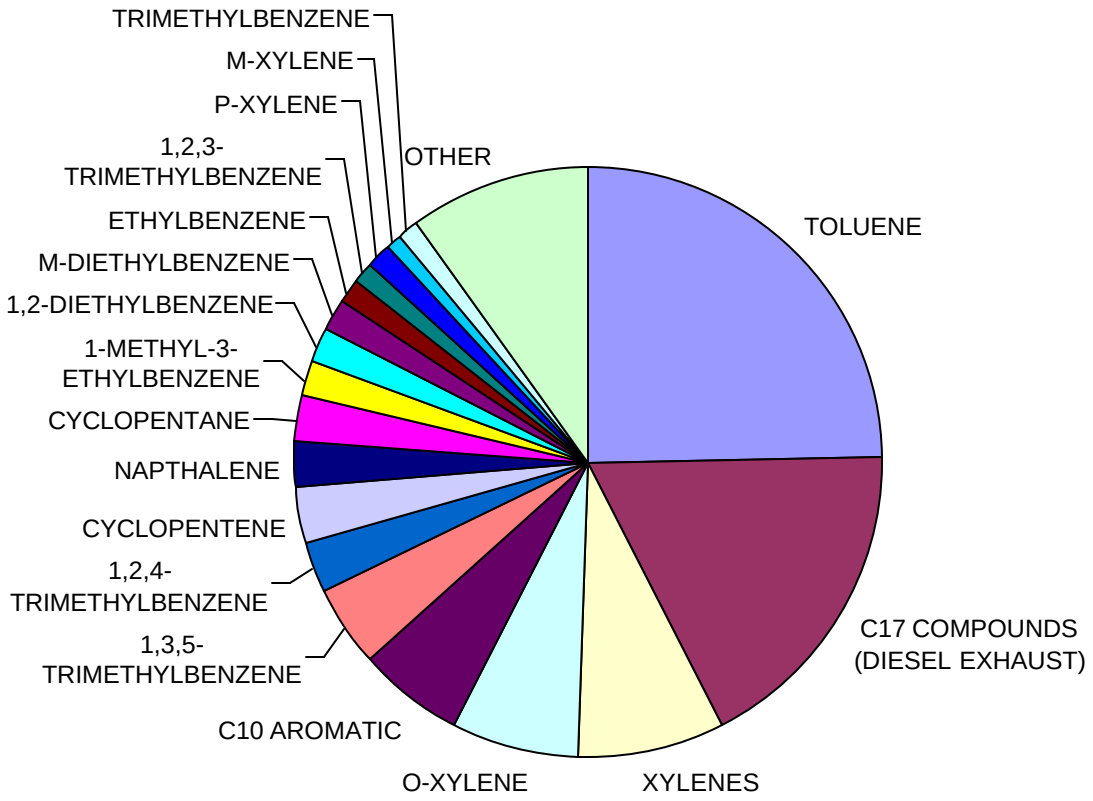
- Point Sources: TCEQ speciated point source database for 2000 (peak ozone day emissions)
- Area/Offroad Mobile: Total VOC estimates from 1999 National Emissions Inventory (NEI). Speciation profiles from TCEQ and SPECIATE3.2
- Onroad Mobile: Total VOC emissions from county-level MOBILE 5. Speciation profiles from Houston area tunnel study (Washburn Tunnel)
- $SOA_i = FAC_i * emissions_i * \text{'fraction reacted'}_i$

  FAC and typical 'fraction reacted' from literature (Grosjean and Seinfeld, 1989, Grosjean 1992)

VOC Emissions Totals (tons/day)

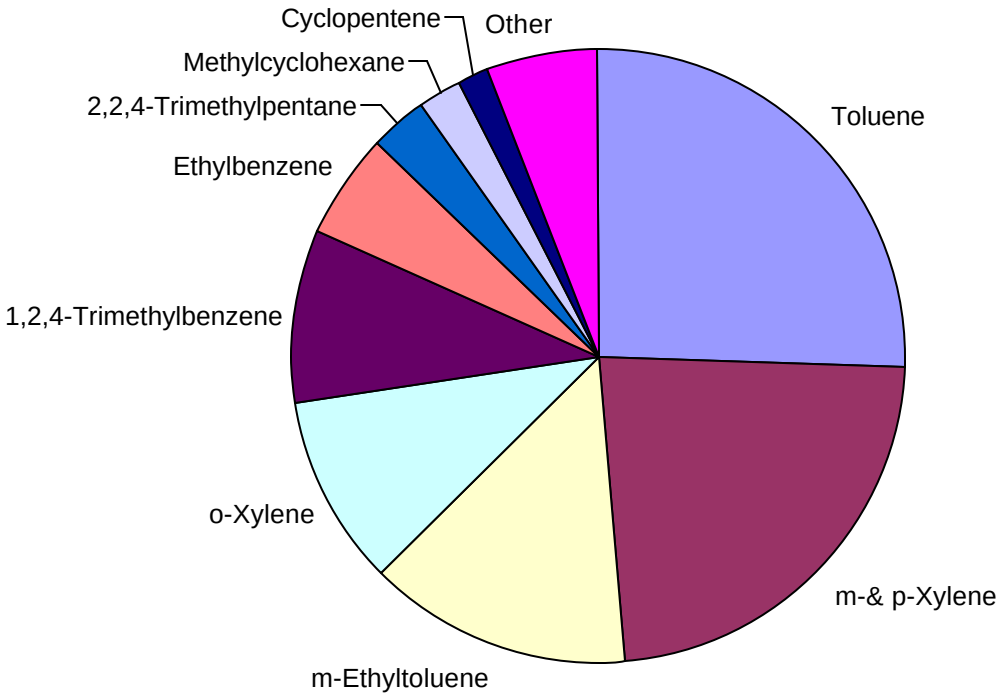
	Point	Area/Offroad Mobile	Onroad Mobile
Total Emissions	226	559	246
Speciated Emissions	217 (96%)	462 (83%)	246 (100%)
SOA Precursor Emissions	44 (20%)	150 (27%)	73 (30%)

Area source SOA by compound. Total = 1160 kg/day



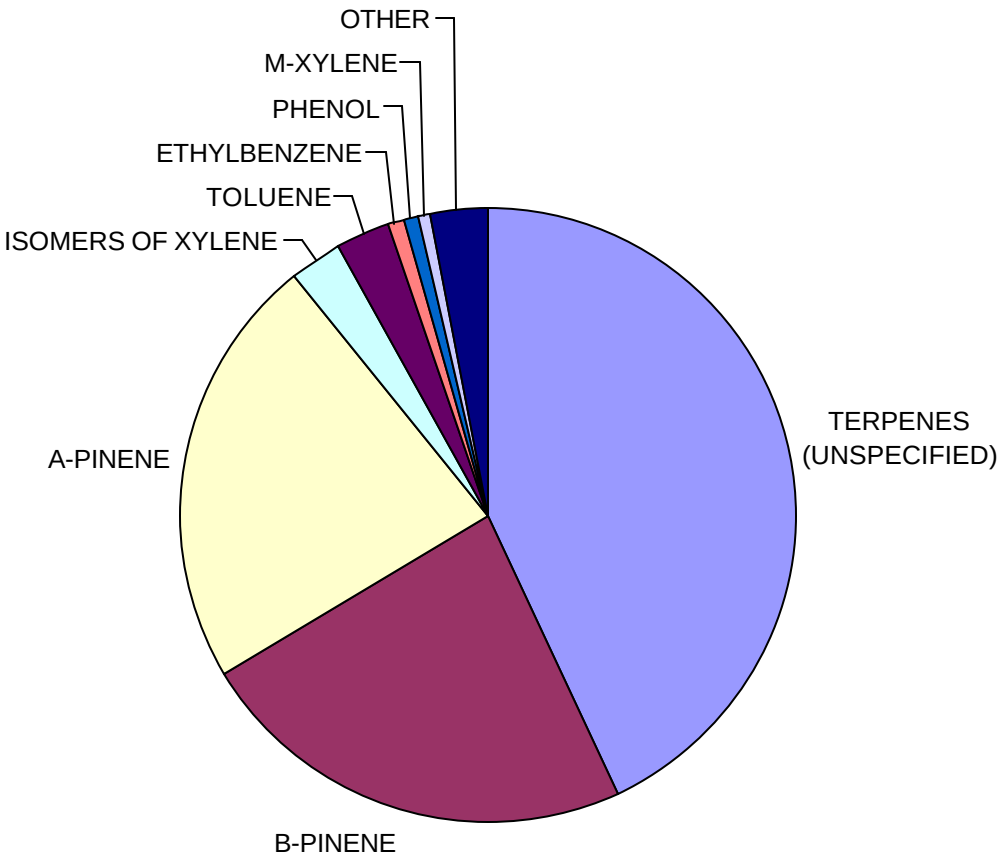
Area and offroad source category	SOA (kg/day)
Construction and Mining Equipment	130
Lawn and Garden Equipment - 2 stroke gasoline	113
Architectural Coatings	109
Lawn and Garden Equipment - 4 stroke gasoline	104
Pleasure Craft - 2 stroke gasoline	83
Industrial Equipment	46

Mobile source SOA by compound. Total = 270 kg/day



Onroad Mobile source category	SOA (kg/day)
Light Duty Gasoline Vehicles (LDGV)	142
Light Duty Gasoline Trucks 1 & 2 (M6) = LDGT1 (M5)	61
Light Duty Gasoline Trucks 3 & 4 (M6) = LDGT2 (M5)	25
Heavy Duty Gasoline Vehicles 2B thru 8B & Buses (HDGV	17
All HDDV including Buses	17

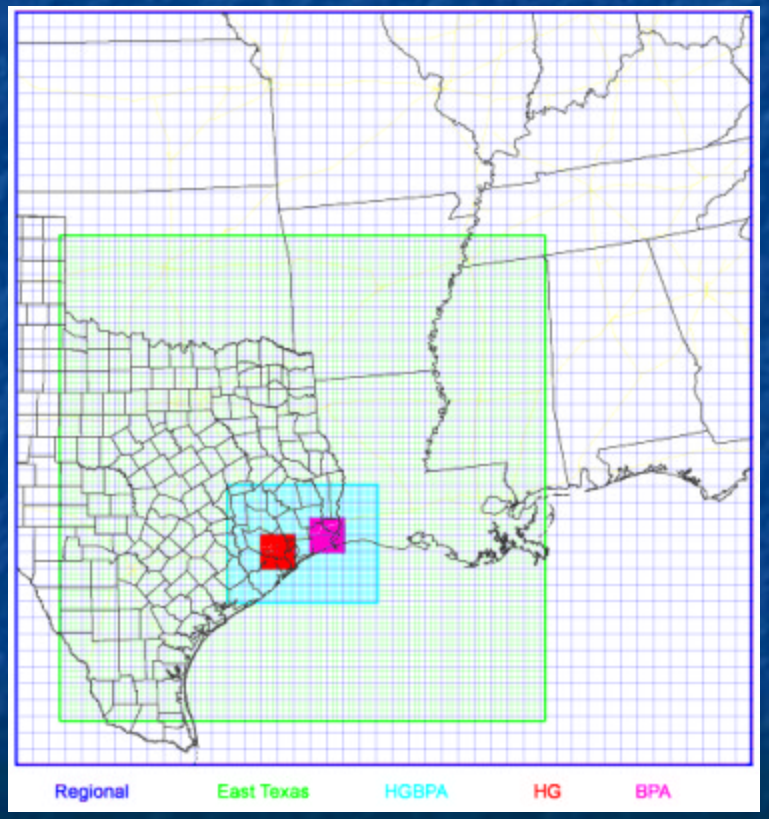
Point source SOA by compound. Total = 1580 kg/day



Point source category	SOA (kg/day)
Pulp and Paper and Wood Products	1406.2
Petroleum Industry	45.2
Petroleum Product Storage at Refineries	43.5
Chemical Manufacturing	38.9
Surface Coating Operations	23.5

SOA formation 2: Photochemical Modeling

- 'TXAQS' Episode 8/25/2000-9/1/2000
- Comprehensive Air Quality Model w Extensions (CAMx), modified to include:
  - SAPRC99 mechanism for SOA precursors
  - Module to predict SOA formation
  - Emissions re-processed into new model species including biogenic monoterpenes



Chemical Mechanism

- SAPRC99 fixed parameter mechanism with:
  - α-pinene, β-pinene, sabinene, limonene, Δ^3-carene represented explicitly
  - High-SOA yield, low-SOA yield and no-SOA yield aromatic species represented separately
  - Texas anthropogenic emissions profile for parameters of lumped model species
- Extensive source code modifications to CAMx 3.1 and SAPRC99 source code for solution of new mechanism with Implicit-Explicit Hybrid solver.

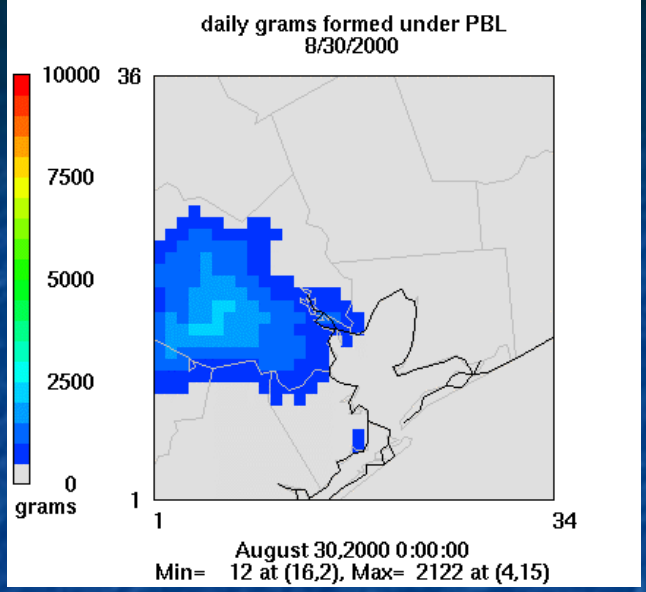
SOA model

- Model based on gas/particle partitioning yields (Odum et al. 1996):

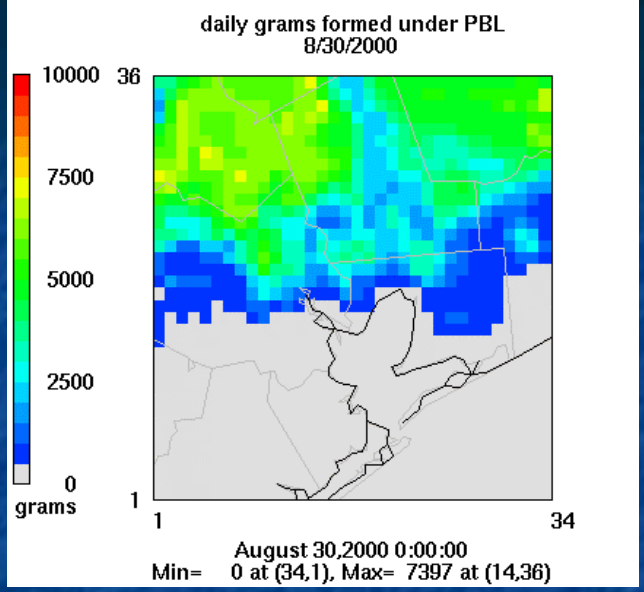
$$\Delta SOA = \Delta HC * Y = \Delta HC * M_o \left(\frac{\alpha_1 K_{om,1}}{1+K_{om,1} M_o} + \frac{\alpha_2 K_{om,2}}{1+K_{om,2} M_o} \right)$$

- Mo inputs from spatially interpolated ambient measurements of total organic carbon.
- K coefficients adjusted to account for temperature of model grid cell.
- Total mass of SOA formed under PBL calculated at each hour, in each grid column, for each precursor reaction: high-SOA and low-SOA yield aromatics with OH, five explicit monoterpenes with OH, O_3 and NO_3

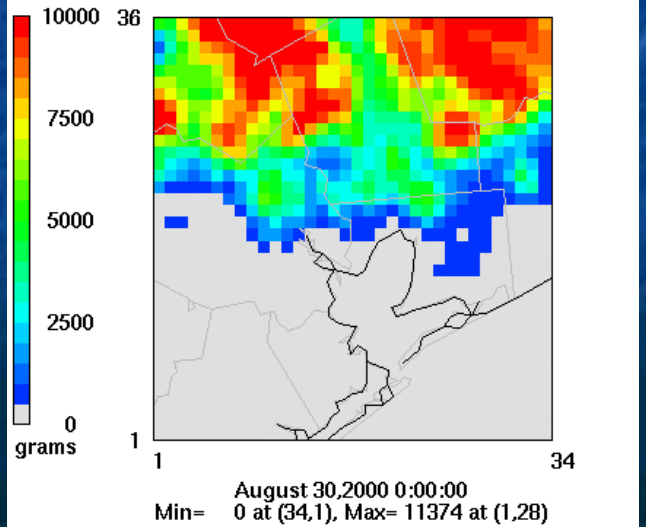
SOA formation; aromatics w OH



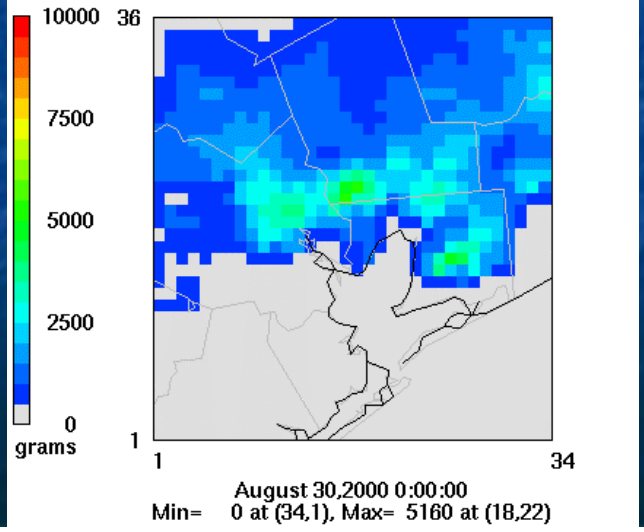
SOA formation; mterpenes with OH



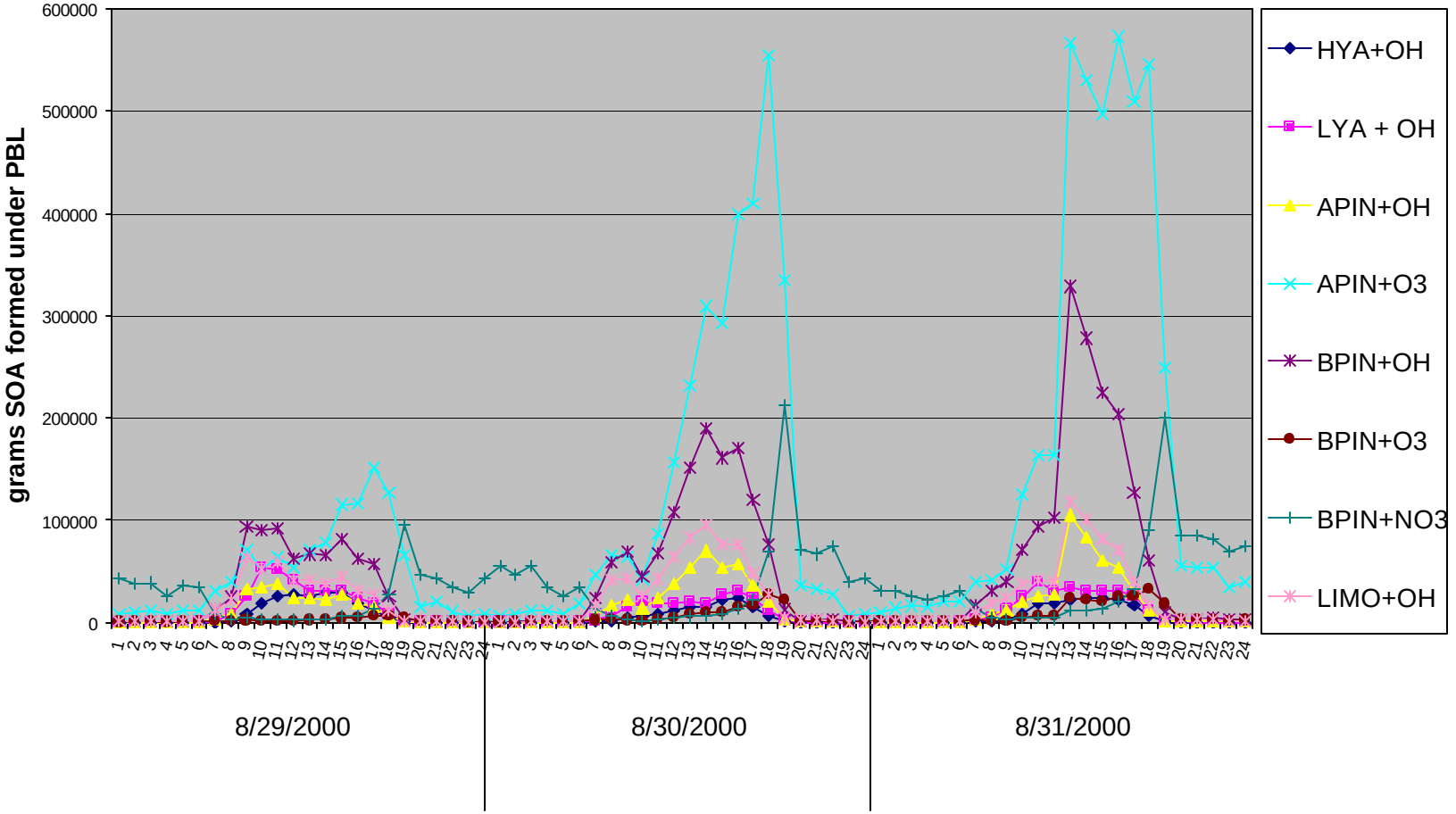
SOA formation; mterpenes with O3



SOA formation; mterpenes with NO3



SOA formation through individual reaction pathways



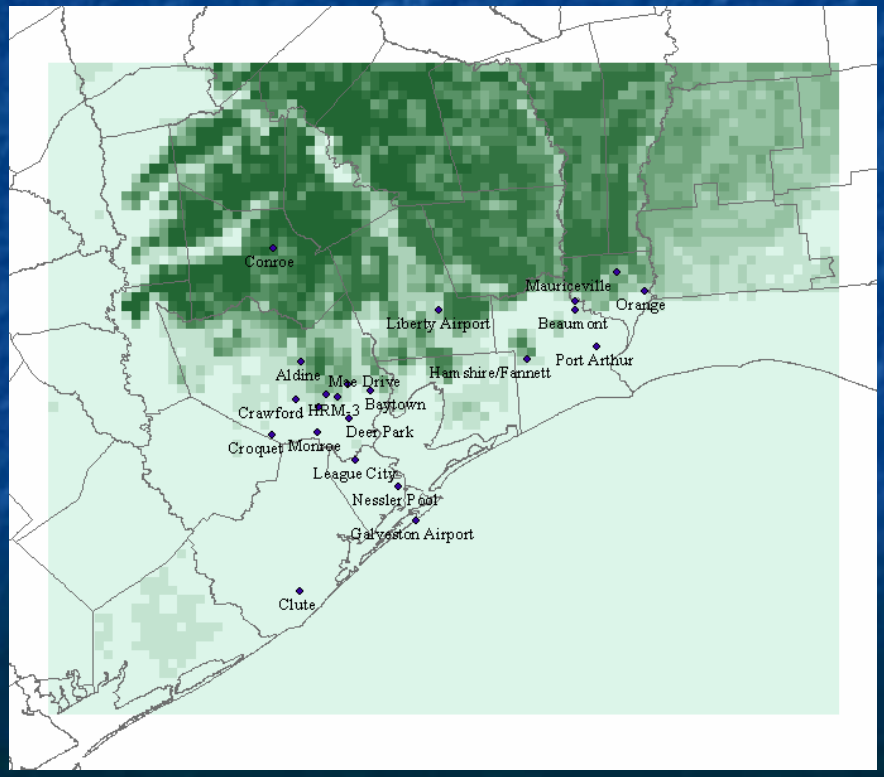
Conclusions

- Current emissions inventories show that biogenic monoterpenes dominate SOA formation in Southeast Texas.
- Aromatic precursors account for the majority of SOA formation in urban Houston, and come from area, offroad, onroad and point sources.
- Point source monoterpene emissions may also be important SOA precursors.

Biogenic SOA

- Speciation data for individual monoterpenes was compiled by tree species (Geron et al. 2000)

α-pinene emissions



ocimene emissions