Houston Triangle Data Analysis and Source Apportionment

Proposed Analysis for the September 5-27 2006 Campaign

Carl Berkowitz, Liz Alexander, YuLong Xie and Xiao-Ying Yu
Battelle Northwest Laboratories, Richland, WA

Tom Jobson
Washington State University, Pullman, WA

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A Review of the 2006 Campaign

- **Final report is at**

  http://files.harc.edu/Projects/AirQuality/Projects/H075/H075FinalReport.pdf

- **Objective:**
  - **make co-located VOC/aerosol observations at the Aldine, Deer Park and Bayland Park air monitoring stations during the TexasAQS II study (2006)**
  - **Locations selected based on ease of access and past measurements showing high ozone design values + contrasts in aerosol composition and hygroscopicity.**

A Review of the 2006 Campaign

- A 4-week campaign carried out during September 2006 to provide continuous observations of hydrocarbons, aerosols, and selected trace-gases at the Deer Park, Aldine, and Bayland Park air monitoring stations in Houston, Texas.

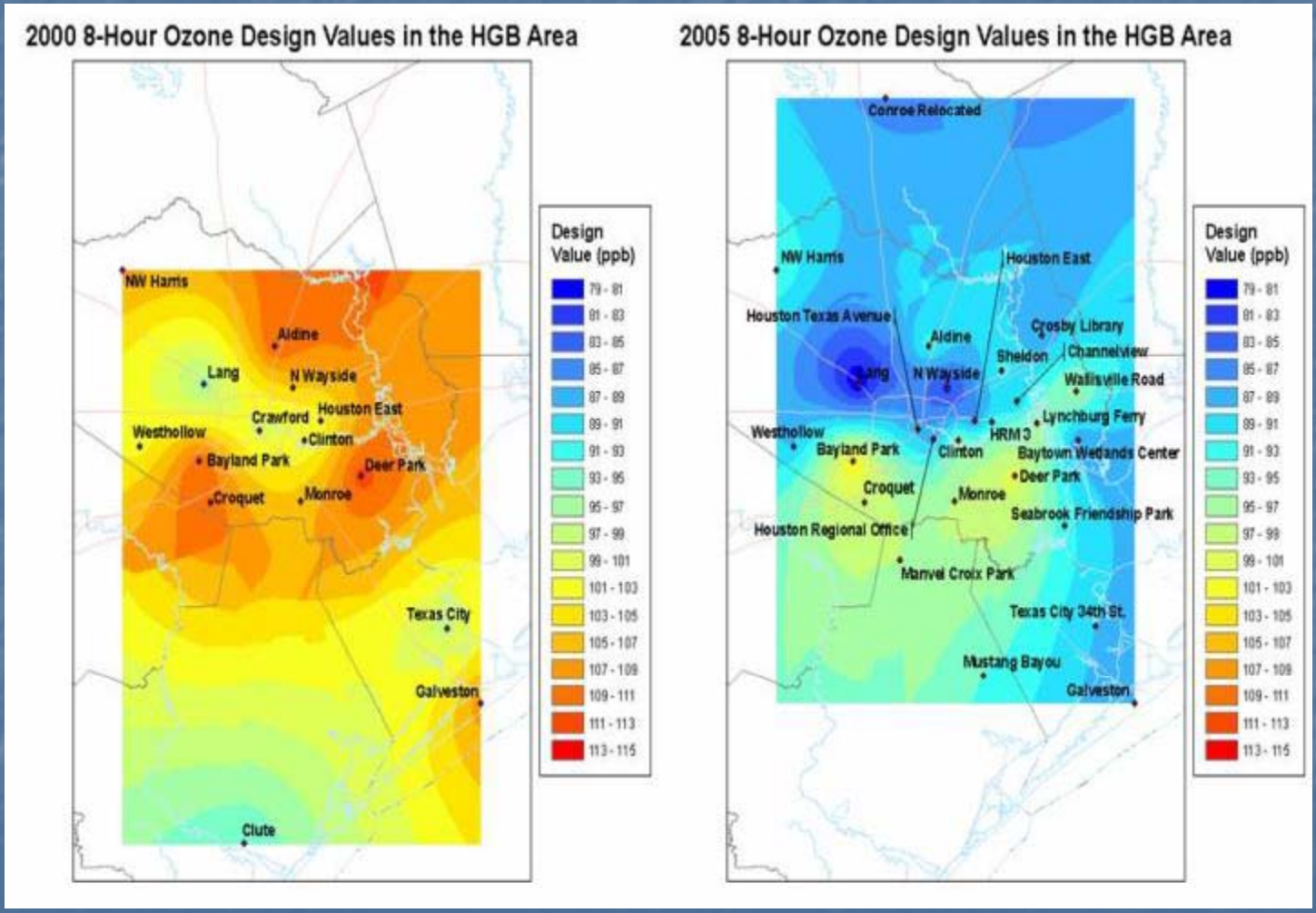
- Key Instruments at each site:
  - Three Aerodyne Aerosol Mass Spectrometers
  - Two Proton-Transfer Reaction Mass Spectrometers (Battelle & WSU)
  - One Proton-Transfer Reaction Mass spectrometers (Texas A&M, under separate contract).

- No analysis has yet been done on these observations!

The Houston Triangle

- The PTR-MS measured 22 NMHC
- The AMS measured aerosol composition and size (~40 nm -~800 nm)
- Resulted in an almost continuous set of co-located VOC/aerosol observations at three TCEQ air monitoring stations
  - Aldine: urban emission sources and transported emissions from Ship Channel
  - Deer Park: upwind of Houston Ship Channel under S. flow
  - Bayland Park: west side of city

Triangle Sites are in Chemical Hot Spots



(Figures courtesy of the TCEQ Data Analysis Team)

Trailer Delivery, Aldine Site

Inlet Installation,
Deer Park Site

Bayland Park Site

Instruments Deployed during the Campaign

Measurement	Deer Park	Bayland Park	Aldine	Data Source
Aerosol Mass Spec.	×	×	×	PNNL/EMSL
PTR-MS	×	×	×	Battelle/WSU/TA&M
Canisters	×	×		WSU
O3	×	×	×	Battelle/WSU/TCEQ
CO	×	×	×	Battelle/WSU/TCEQ
NO/NO2/NOx	×	×	×	Battelle/WSU/TCEQ
SO2	×	×		Battelle/WSU
TDMA	×	×	×	TA&M
Ceilometer	×			Battelle
PM2.5 mass	×	×	×	TCEQ
GC for HC	×	×	×	TCEQ
Met data	×	×	×	TCEQ

Proposed Analysis

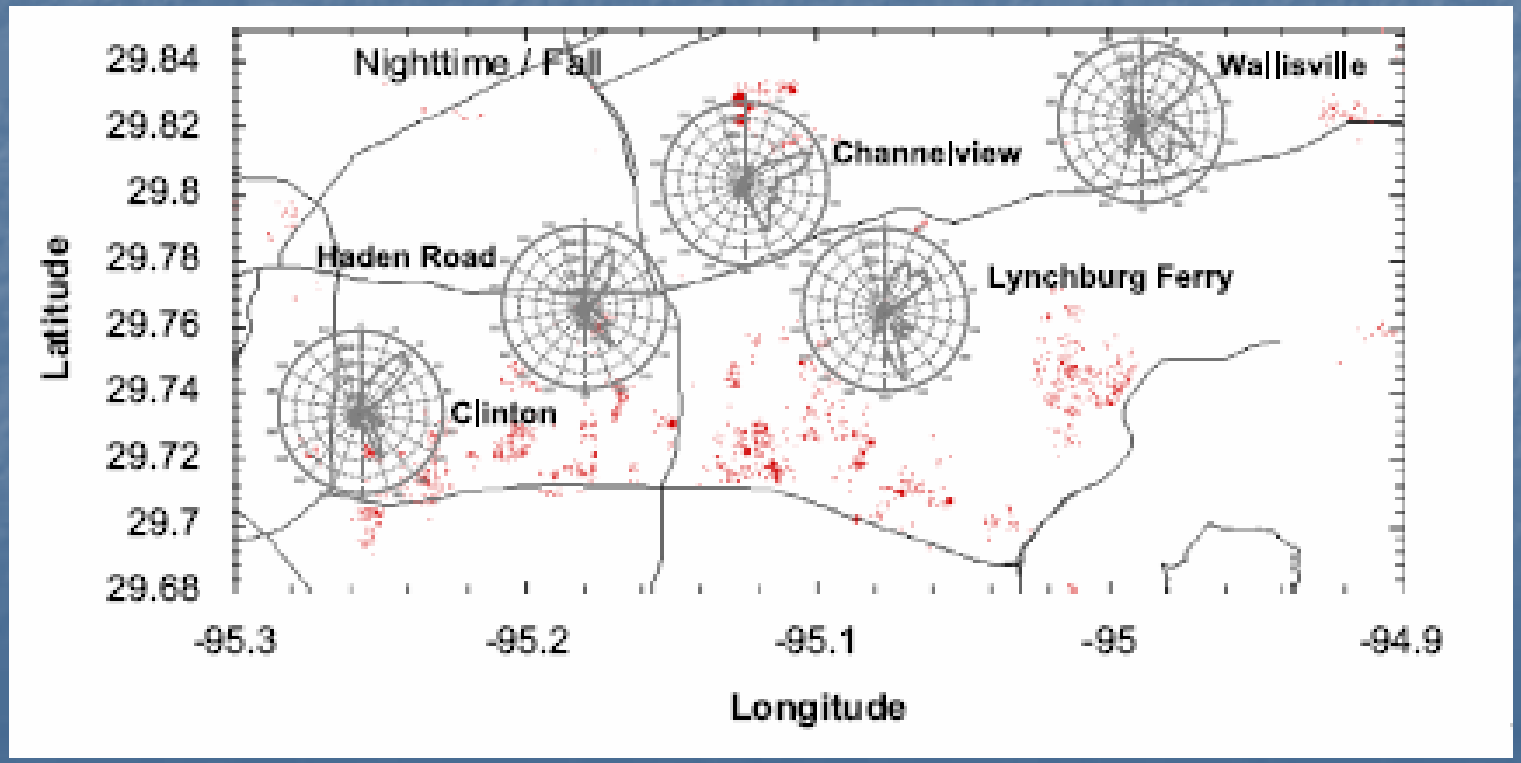
- **Task I: Statistical Overview:**
- **Task II: Identification of Key Source Regions:**
- **Task III: Consistency of Inventory with Measurements:**

Task I: Statistical Overview

- Develop summary statistics for each measured VOC at each site.
- Focus attention on the outliers, or “high” values.
  - Can we identify common groups of compounds?
  - Do they have a common source region?
- Prepare summary tables and discussion relating means, medians, variance, etc.

Task II: Identification of Key Source Regions - I

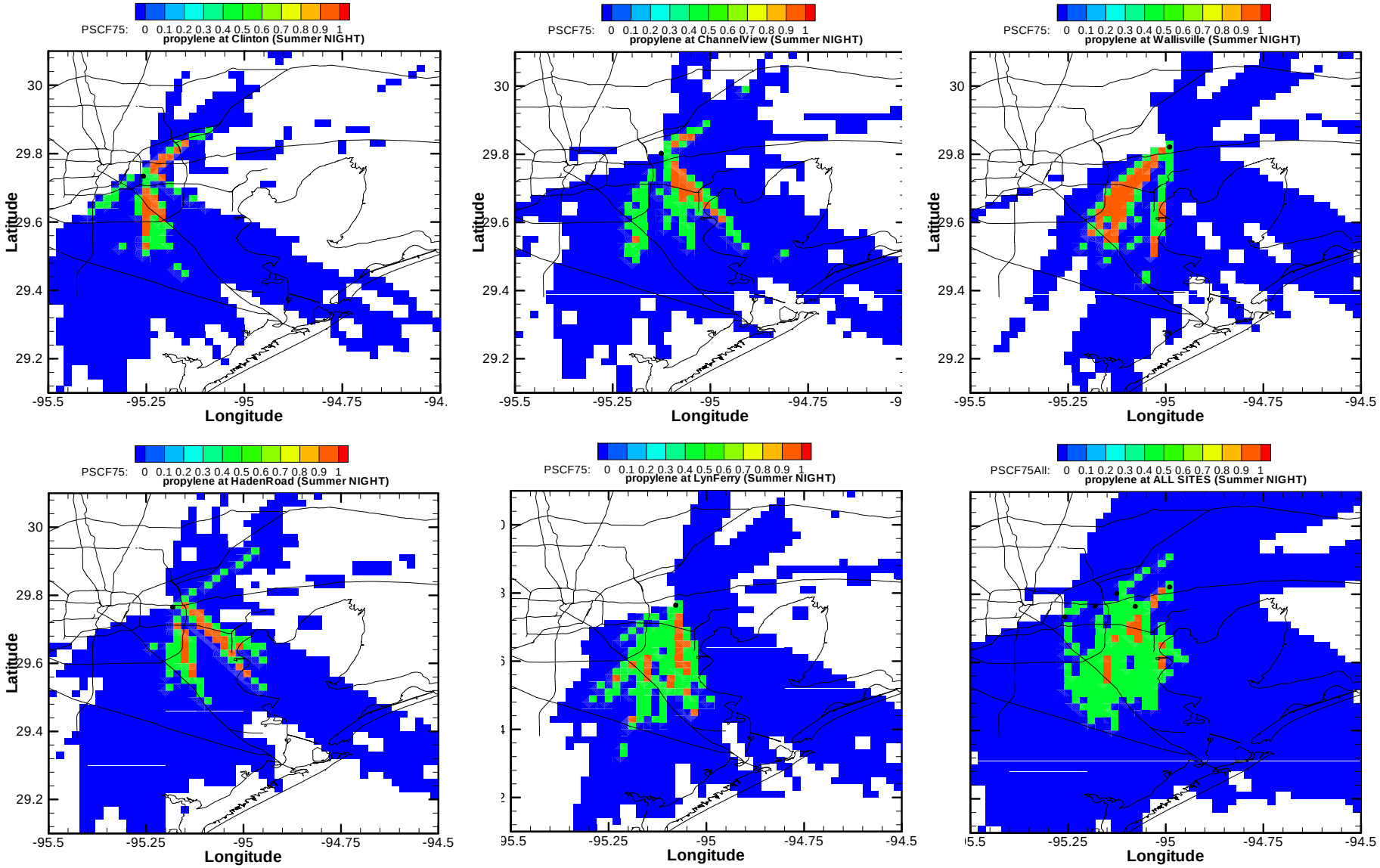
- I) Conditional Probability Functions combine directional information with high concentrations of VOCs
  - defined as ratio of the number of samples in the wind sector y with mixing ratios greater than some ‘‘high’’ concentration, to the total number of samples in the same wind sector.



Task II: Identification of Key Source Regions - II

- II) Potential Source Contribution Function analysis:
  - Based on time series of the location of simulated air parcels released from each of the Triangle sites.
  - Associates each back trajectory with an observation at a given receptor site and evaluates the time of the arriving parcel at points along its back trajectory.
  - Results in a map showing the probability of a given cell being associated with an elevated measurement at the receptor site of interest.

Example: Potential Source Contribution Functions



Task III: Consistency of Inventory with Measurements:

- **Are TCEQ emissions inventories consistent with concentrations of corresponding species measured by the PTR-MS and canisters during the Triangle Campaign?**
  - **Ambient ratio analysis**
    - **Key Idea: the confidence in the inventories is assessed by comparing ratios of measured concentrations to the assumed emissions of the corresponding species within the inventory**
    - **e.g., (ambient CO/ambient NMHC)/(emission CO/emission NMHC)**
    - **CO: ppm, NMHC: ppm-carbon**
  - **Strengths:**
    - **Ratios are less influenced by day-to-day variations in insolation, transport, etc.**
    - **Don't need absolute concentrations: relatively robust technique**
  - **Weaknesses:**
    - **Little information on actual magnitude of emissions**
    - **Not so good for photochemically active pollutants**
    - **Difficult to assess if discrepancy associated with numerator or denominator**

The 23 Masses That Were Monitored by PTR-MS and Their Nominal Identification:

Mass	Compound	Formula
M33	methanol	CH_3OH
M35	hydrogen sulfide	H_2S
M42	acetonitrile	C_2H_3N
M43	propene	C_3H_6
M45	acetaldehyde	C_2H_4O
M47	ethanol	C_2H_6O
M57	butenes	C_3H_6O
M59	acetone	C_3H_6O
M61	acetic acid	$C_2H_4O_2$
M63	dimethyl sulfide	C_2H_6S
M69	isoprene	C_5H_8

Mass	Compound	Formula
M71	MVK+MACR +pentenes	C_4H_6O, C_5H_{10}
M73	MEK	C_4H_8O
M79	benzene	C_6H_6
M93	toluene	C_7H_8
M95	phenol	C_6H_6O
M105	styrene	C_8H_8
M106	isopropyl nitrate	$C_3H_7NO_3$
M107	xylenes	C_8H_{10}
M109	cresols	C_7H_8O
M121	C3-benzenes	C_9H_{11}
M135	C4 benzenes	$C_{10}H_{14}$
M137	Mono-terpenes	$C_{10}H_{16}$

Expected Benefits to Come from an Analysis of the Houston Triangle Observations

- Focus of this analysis will be on “high” values
  - Which compounds?
  - Which groups of compounds?
  - What is their source area?
- Which areas in Houston, as defined by a high-resolution grid, are associated with “high” values?
- DOE/PNNL interested in aerosol component and may provide independent support for study of VOCs and aerosol characterization.