Highlights from the 2010 American Meteorological Society Meeting

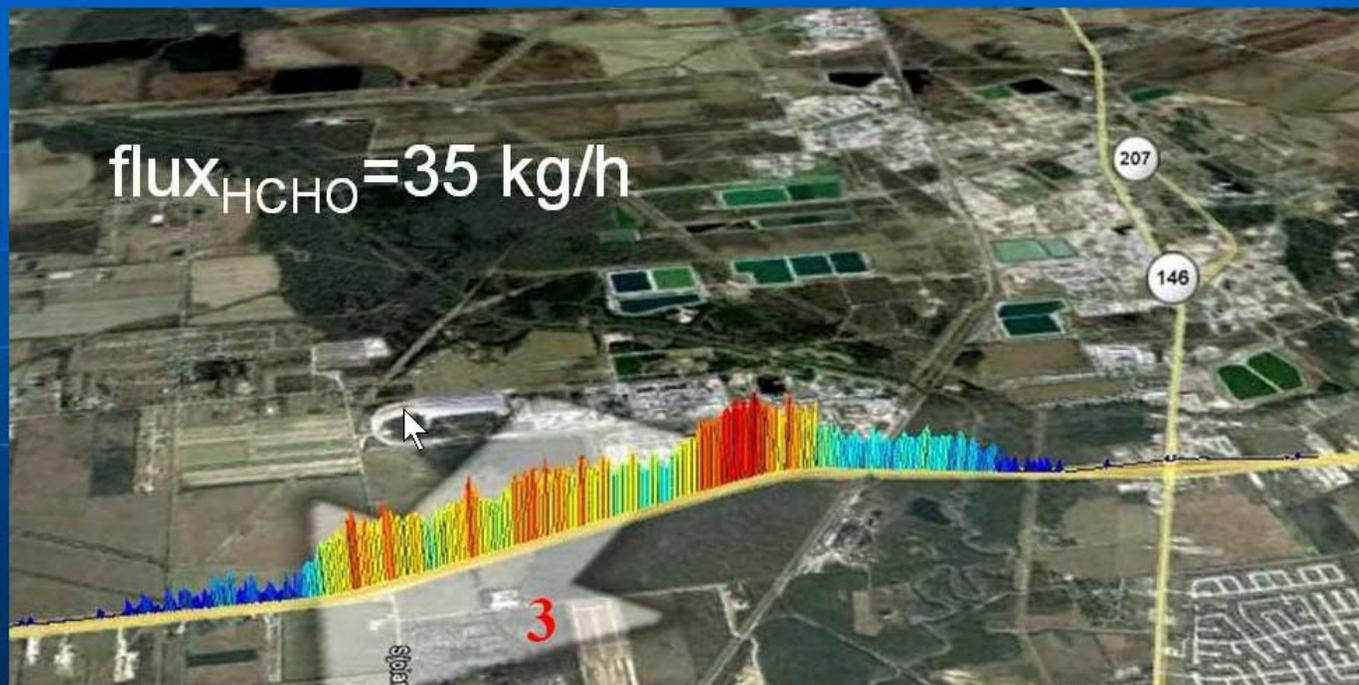## Jim Smith and Mark Estes
Southeast Texas Photochemical Modeling Technical Committee Meeting

April 7, 2010

SOF and mobile DOAS measurements during "TEXAQS 2009" *(he really means "SHARP")*

Johan M. Mellqvist, Chalmers University of Technology, Gothenburg, Sweden

# SOF and mobile DOAS measurements during "TEXAQS 2009"

- For the Houston Ship Channel, 2009 alkene (olefin) emissions were lower than 2006 emissions; Mont Belvieu and Texas City emissions were similar

- 2009 alkane emissions from HSC & Texas City were similar to 2006, Mont Belview emissions higher

- Primary formaldehyde emissions of 15-30 kg/hour were found in close-by measurements at several sites

- Poor correlation of CO and alkenes downwind of main alkene sources identified by SOF implies most emissions are from fugitives, not flares.

Olga Pikelnaya, UCLA

- Measurements of formaldehyde during SHARP

- MAX-DOAS upwind-downwind experiment at Texas City

- Estimated HCHO flux of 720 kg/hour—much higher than Mellqvist 15-30 kg/hour, from the same area.

- Obviously some disagreement between methods.

Ezra Wood, Aerodyne (H113)

- Aerodyne mobile monitoring van sampled NOx, SO2, CO, formaldehyde, alkenes during SHARP study at Texas City, Mont Belvieu, Ship Channel area
- SCIPUFF inverse model used to estimate location and strength of emission sources
- Mt Belvieu measurements:
  - Ethene: 1.07 kg/hr, 22.2 kg/hr, 150 kg/hr
  - Propene: four sources from 0.7 – 10.3 kg/hr
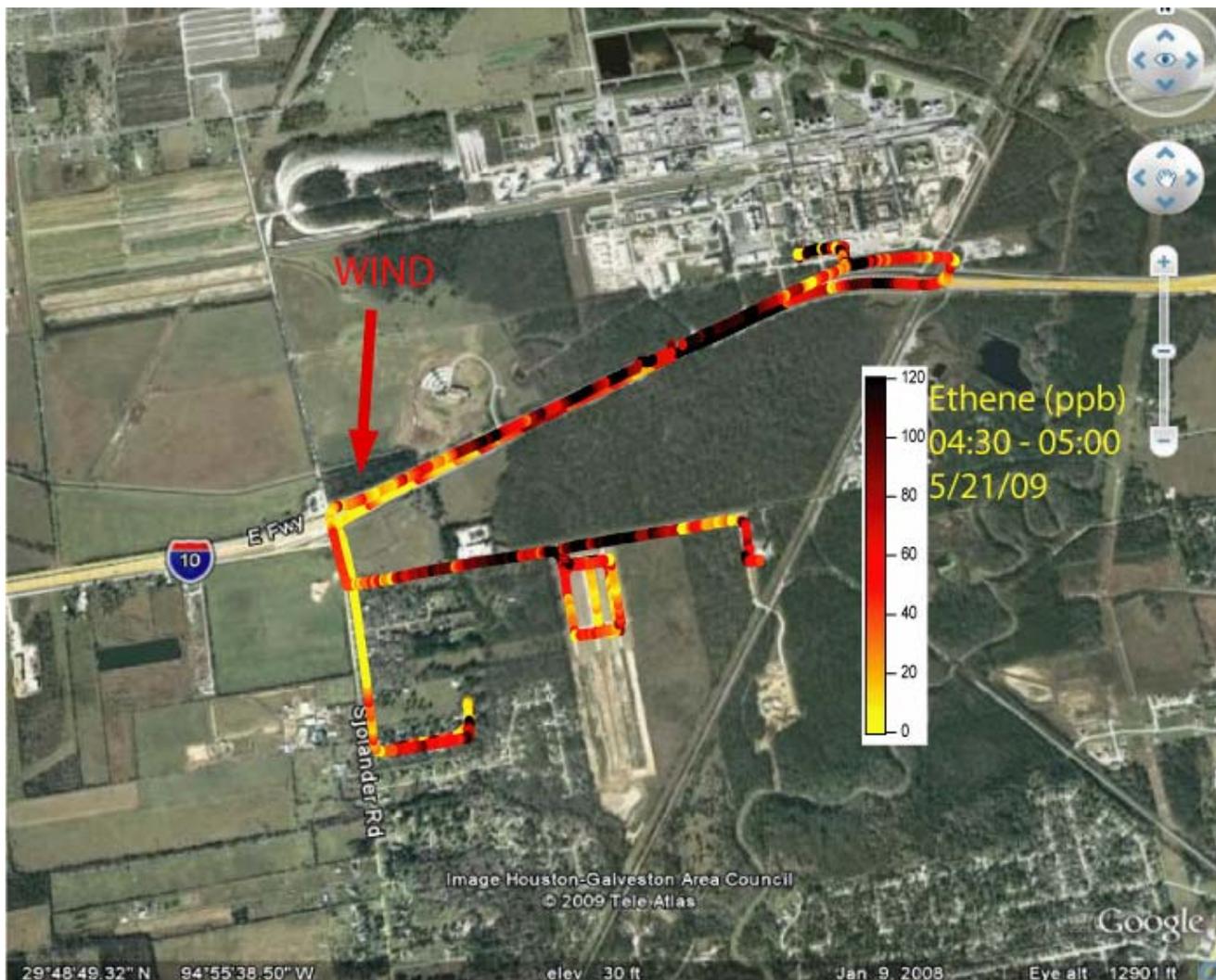
An example of Aerodyne van sampling of Chevron-Mt Belvieu plumes.
Darker colors indicate higher concentrations.

Traffic related emissions of HONO and HCHO in Houston, TX

Bernhard Rappenglueck, et al, Univ. of Houston

- Sampling site @ US 59 and SW IH 610 (near Galleria)

- Preliminary analysis based on subset of data collected

- Observed elevated HONO during daytime (~600 pptv)

- 4 pptv HCHO/ppbv CO; R^2=0.48
- 2 pptv HONO/ppbv CO; R^2=0.632
- 100 pptv HONO/ppbv NO_2; R^2=0.70
- 19 pptv HONO/ppbv NO_X; R^2=0.40

Imaging of point source emissions of HCHO and SO2 in Houston, TX, using Differential Optical Absorption Spectroscopy

Jochen Stutz, University of California, Los Angeles

- Portable DOAS, up to 10 hours on 3 car batteries
- Nice images of HCHO in flare flames
  - Many, but not all burning flares show HCHO
- HCHO hangs over petrochemical facilities
  - Probably mostly secondary
- Little HCHO observed in ship exhaust

Vertical concentration profiles of O3, NO2, SO2, HCHO, HONO, and NO3 during the 2009 SHARP experiment in Houston, TX

Kam Weng Wong, University of California, Los Angeles

- Used Long-Path DOAS installed atop Moody Tower at UH
- Observed vertical gradients at night and on stable days in HONO, HCHO, O3, SO2, NO2, and NO3.
- O3 concentrations increased with altitude, while other pollutant concentrations decreased with altitude.
- 1-D modeling studies reproduced the gradients, but modeled rush-hour HONO too low.

# Impact of lightning-NO emissions on eastern United States photochemistry determined using the CMAQ model

Kenneth E. Pickering, NASA/GSFC

- Lightning NO_X now included in CMAQ
- 60-80% of upper tropospheric NO_X 20-30% of upper tropospheric O_3
- Reduces CMAQ low NO bias in upper troposphere
- Lightning NO_X contributes < 2 ppb to peak 8-hour ozone on 75% of high-ozone days

Improved air quality simulations through the use of GOES-derived cloud data for the TexAQS-II intensive study period

Fong Ngan, NOAA/ERL/ARL

- Found difficulties in correctly simulating air quality for the days with substantial cloudiness and precipitation events
- Cloud related parameters are estimated from GOES data instead of MM5 output processor
- Also update cloud liquid water content based on GEOS data
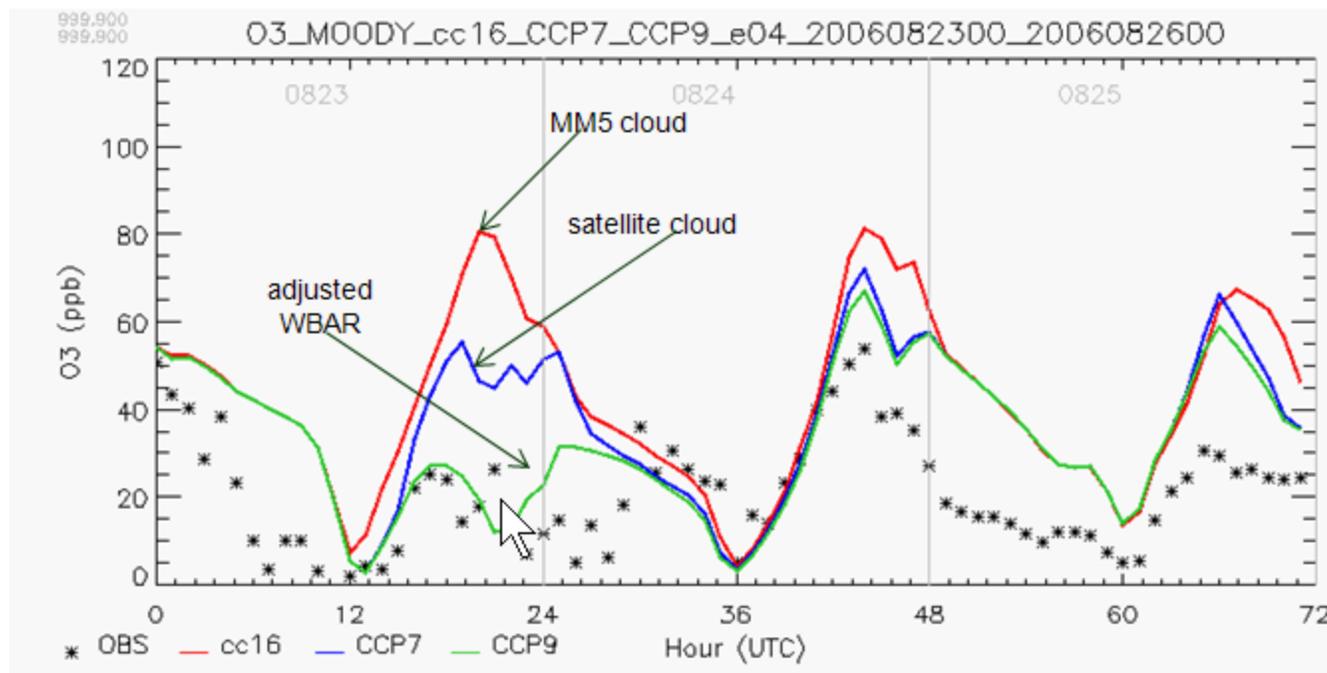
A retrospective analysis of the association of dust storms and respiratory hospitalizations in El Paso, Texas, using a case-crossover study design

Yanlei Peng, University of Texas at El Paso

- El Paso residents are 1.103 times as likely to be hospitalized on a day with dust storms compared to days without, even after adjustment for weather and pollution covariates
- No significant effect by age group, gender, or insurance status

Simulations of nitrous acid for the Houston metropolitan area and comparison with data from the Texas Air Quality Study 2006
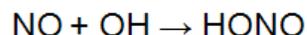
Beata Czader, University of Houston

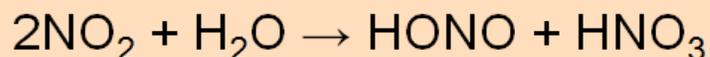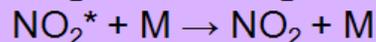## The role of HONO in the atmospheric chemistry

gas phase

$$\boxed{HONO + h\nu \rightarrow OH + NO}$$ morning source of OH

$$NO + OH \rightarrow HONO$$

heterogeneous formation on the surfaces

$$2NO_2 + H_2O \rightarrow HONO + HNO_3$$

CMAQ v. 4.7

current work

$$NO_2 + h\nu \rightarrow NO + O \quad \lambda < 420 \text{ nm}$$
$$NO_2 + h\nu \rightarrow NO_2^* \quad \lambda > 420 \text{ nm}$$
$$NO_2^* + M \rightarrow NO_2 + M$$

$$\boxed{\mathbf{NO_2^* + H_2O \rightarrow HONO + OH}}$$
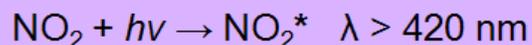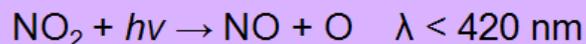
Li *et al.* (2008)
Crowley and Carl (1997)

Simulations of nitrous acid for the Houston metropolitan area and comparison with data from the Texas Air Quality Study 2006

- Heterogenous chemistry in CMAQ increases HONO 10X, closer to observed values
- Relatively small increase in ozone in model
  - HONO deposition very rapid in model
- Largest contribution to HONO formation due to reactions on surfaces
- New reaction $NO_2^* + H_2O \rightarrow HONO + OH$ increases afternoon O_3 but only increases HONO concentrations slightly

Daewon Byun, NOAA

- Forecast modeling with CB05 and CB-IV

- Rural ozone overestimated with CB05

- CB05 includes NOy recycling

- Comparisons show NOy recycling is cause of overestimation, but since NOy recycling is known to occur, the NOy deposition rates must be underestimated.

Xinrong Ren, U Miami

- Measurements of HONO fluxes during May 2009 at UH campus

- TexAQS II observations show HONO is an important OH radical source in Houston

- Model doesn't make enough HONO—what is missing? Try to deduce missing source by measuring fluxes.

- HONO flux peaks at rush hour, but flux continues until afternoon

- HONO correlated with NO2 concentrations

- HONO pollution rose shows highest concentrations with winds from NE (i.e., Ship Channel, Port of Houston, I-45, etc.)

- Other studies have shown vertical HONO gradients, with highest concentrations near the ground, and decreasing with altitude.

Jim Godowitch, EPA

- Dynamic model evaluation for 2002-2006

- Modeling eastern US for each year from 2002 to 2006. Does the model respond to changing emissions as strongly as observations?

- Less response from model than from obs—especially at 95th percentile.

- Why? His hypothesis: In modeling EI, area sources nearly constant, while other NOx sources decrease.