

How Should We Design the TexAQS II-2006 Intensive?

**TERC Science Advisory
Committee**

November 14-15, 2005 Meeting

**HARC/North Harris Montgomery
Community College District**

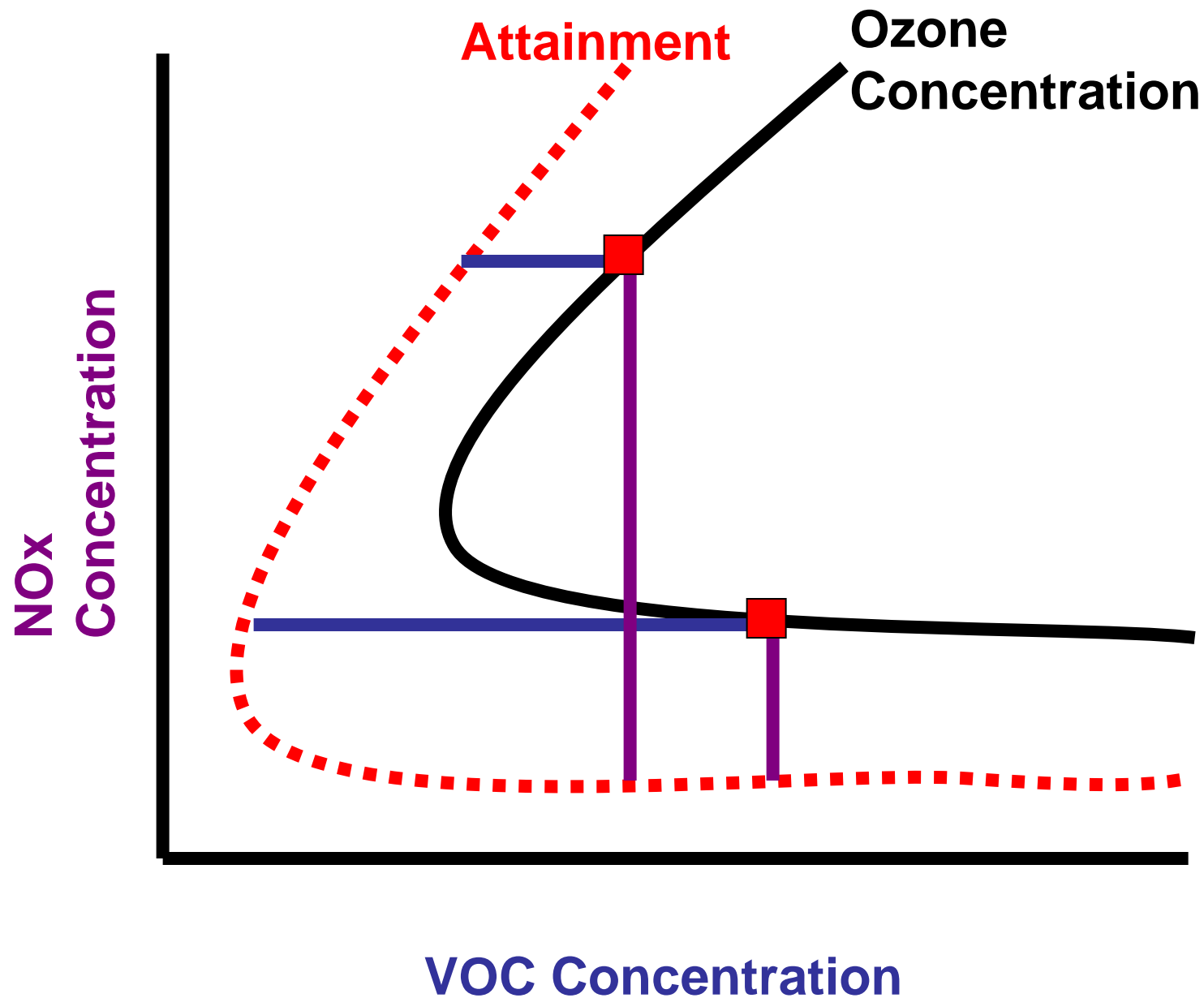
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Outline

- Why do policymakers need models?
- How are the Houston models performing?
- How Should We Design the TexAQS II-2006 Intensive?

Why do policymakers need models?



Model Reliability

- Model must accurately predict precursors and products
- Pollutant concentrations are determined by the interplay of
 - Emissions to the atmosphere
 - Meteorology (dispersion)
 - Chemical reactions (non-linear)
- However, accurate replication of precursors does not guarantee reliability for products (ozone)

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How are the Houston models performing?

- Emissions to the atmosphere
 - Precursor concentrations
- Meteorology
 - Wind vectors
 - CO concentrations
- Chemical Reactions
 - Secondary pollutant concentrations

Model Analysis Material

- Simulation performed by UH
 - X19: UH's QA/QC run of TCEQ's SIP case by **CAMx** (4km run with PSITO2N2 + GOES2 meteorology)
 - Q74: UH's alternative run of X19 by **CMAQ** with UH's the current "best" MM5 run with PSITO2N2 emissions and CMAQ dry deposition
 - Air toxic simulation with expanded SAPRAC mechanism
- Simulations performed by Alpine Geophysics (4km)
 - 1-11 August 2004, 23-31 May 2003, 24 May-4 June 2005, **25-30 September 2004** (Nielsen-Gammon)
 - CAMx, CMAQ, CBIV, SAPRAC
 - All episodes are open source available for all

How are the Houston models performing?

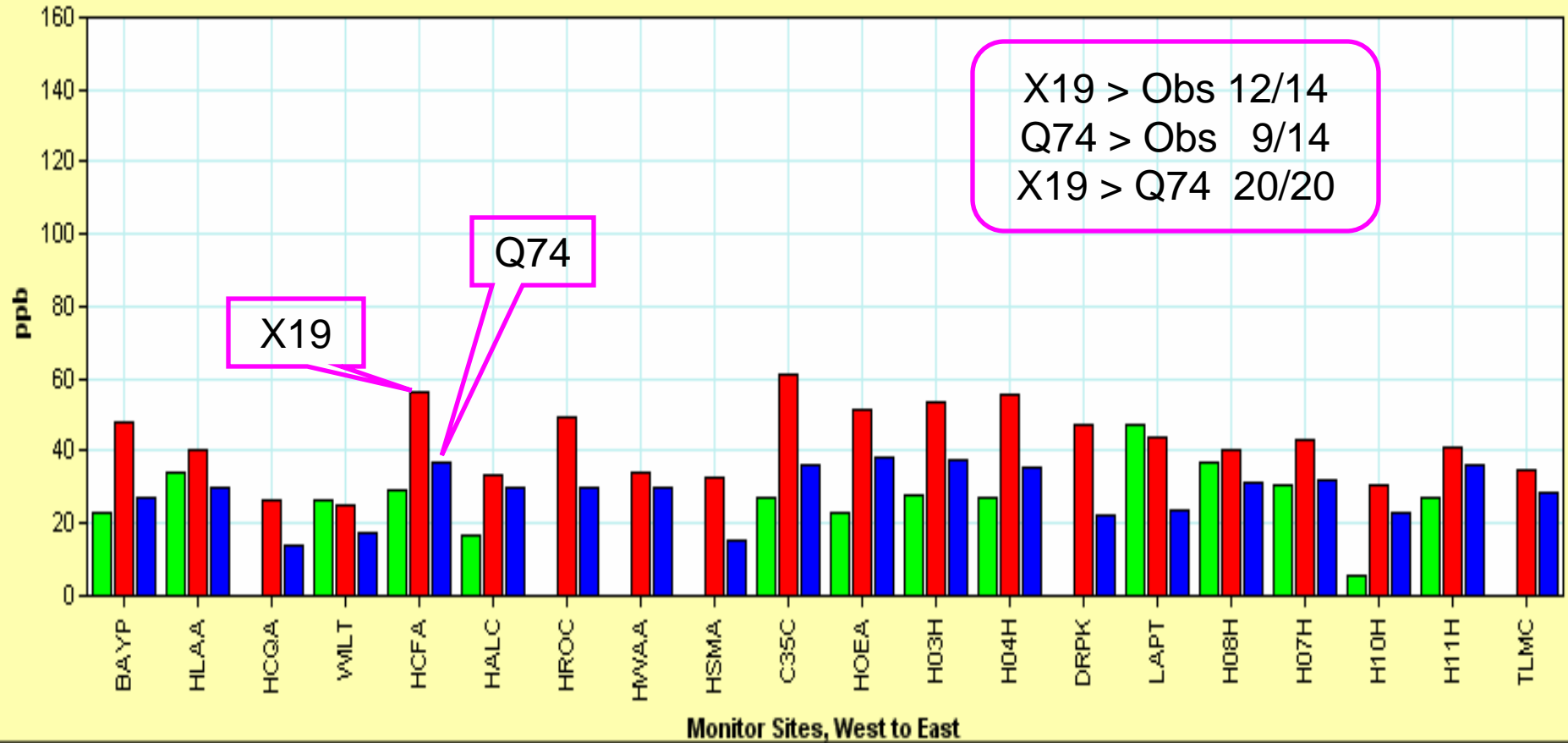
- UH simulation runs
 - Daily peak NO₂ for all surface monitors
 - Time series analysis for ethylene at Clinton (C35C)
 - Time series analysis for CO at Williams Tower
 - Time series analysis for xylene at Clinton(C35)
- Alpine Geophysics simulation runs
 - Neighborhood best 1 hour for NO₂

UH Simulations

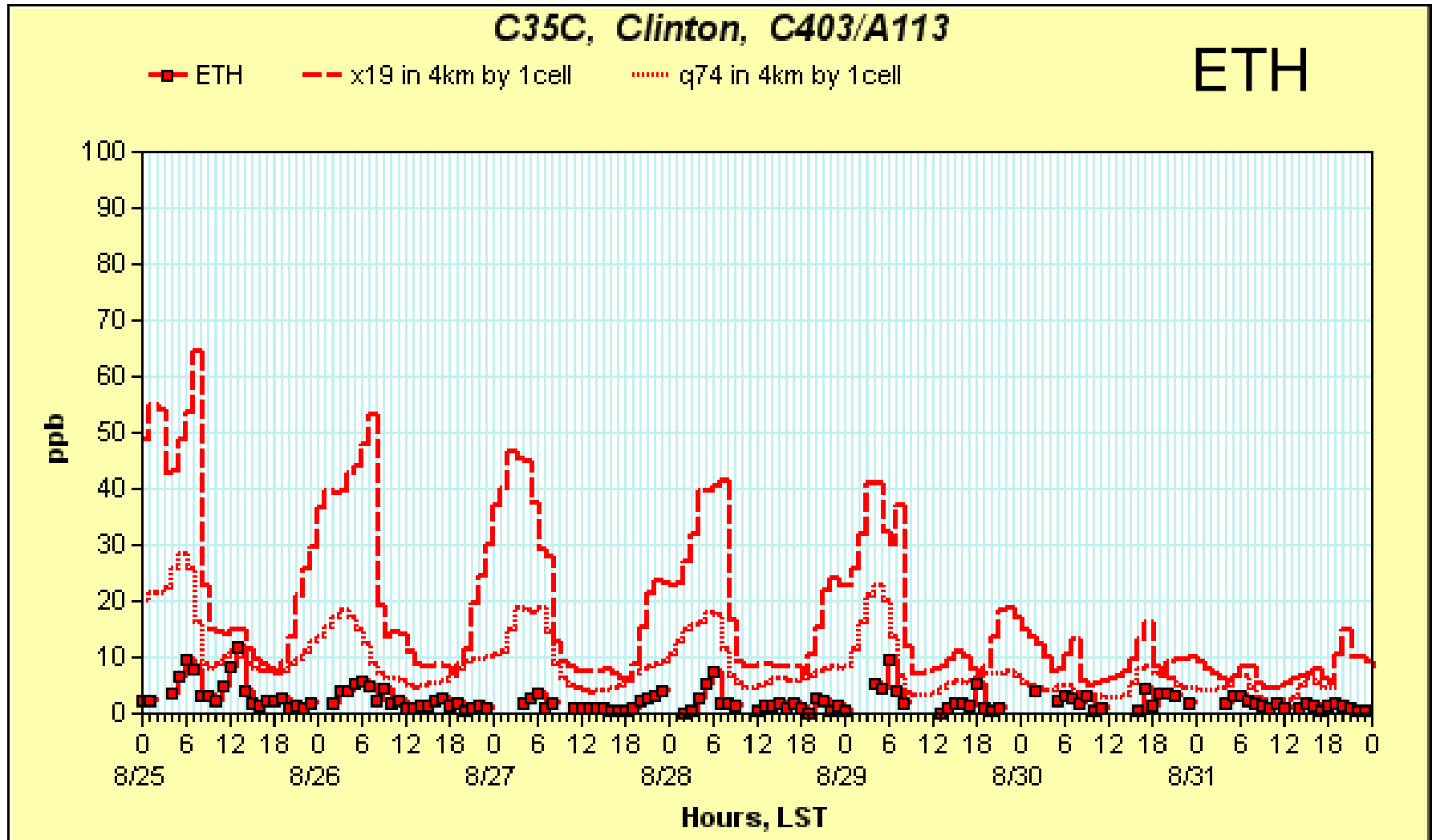
August 25, 2000, Peak NO₂, ppb, 07-17 H

NO₂

Observations x19_4km_1cell_0822_0901 q74_4km_1cell_0823_0831



UH Simulations

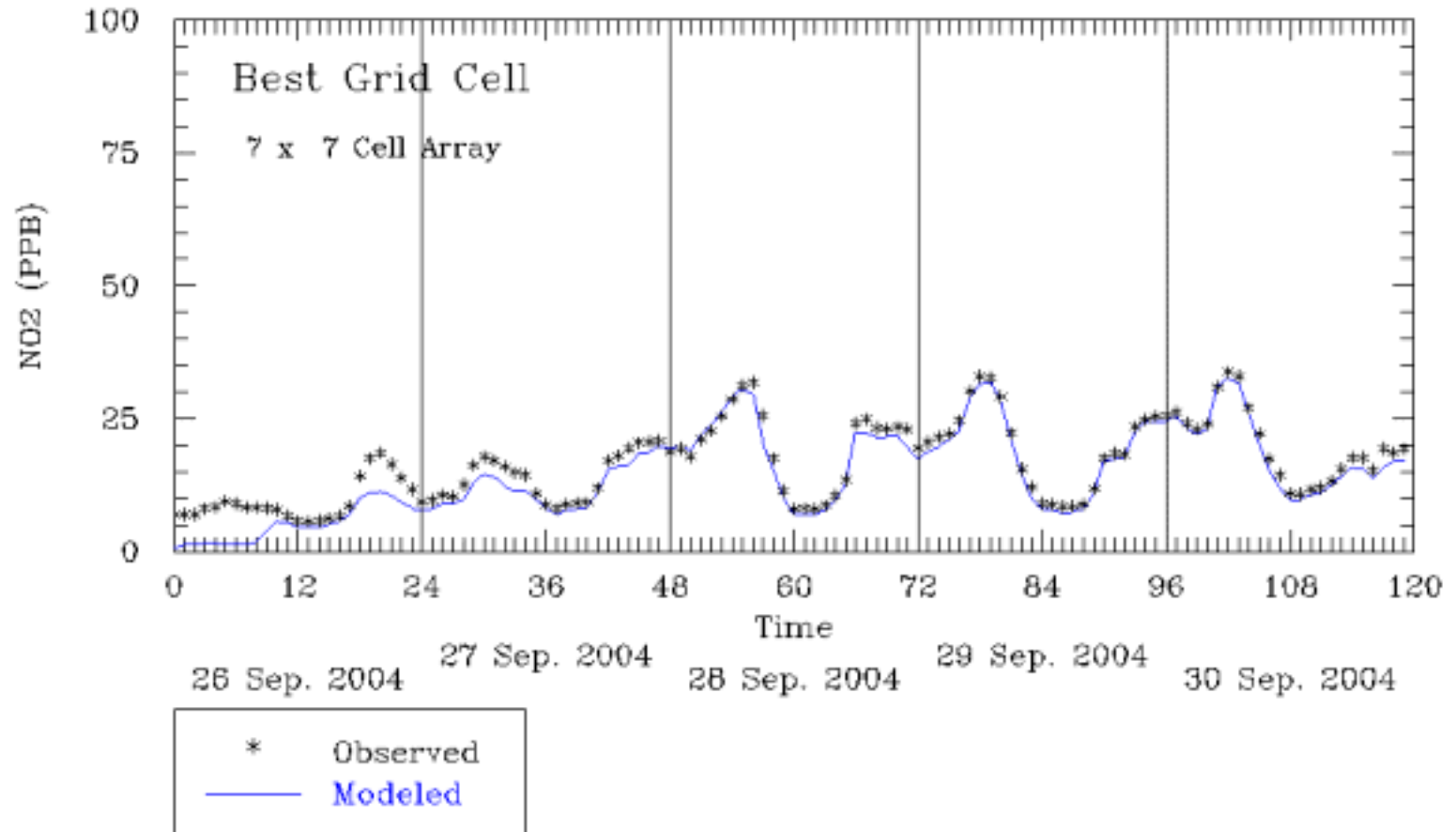


- **Clinton (C35C)**

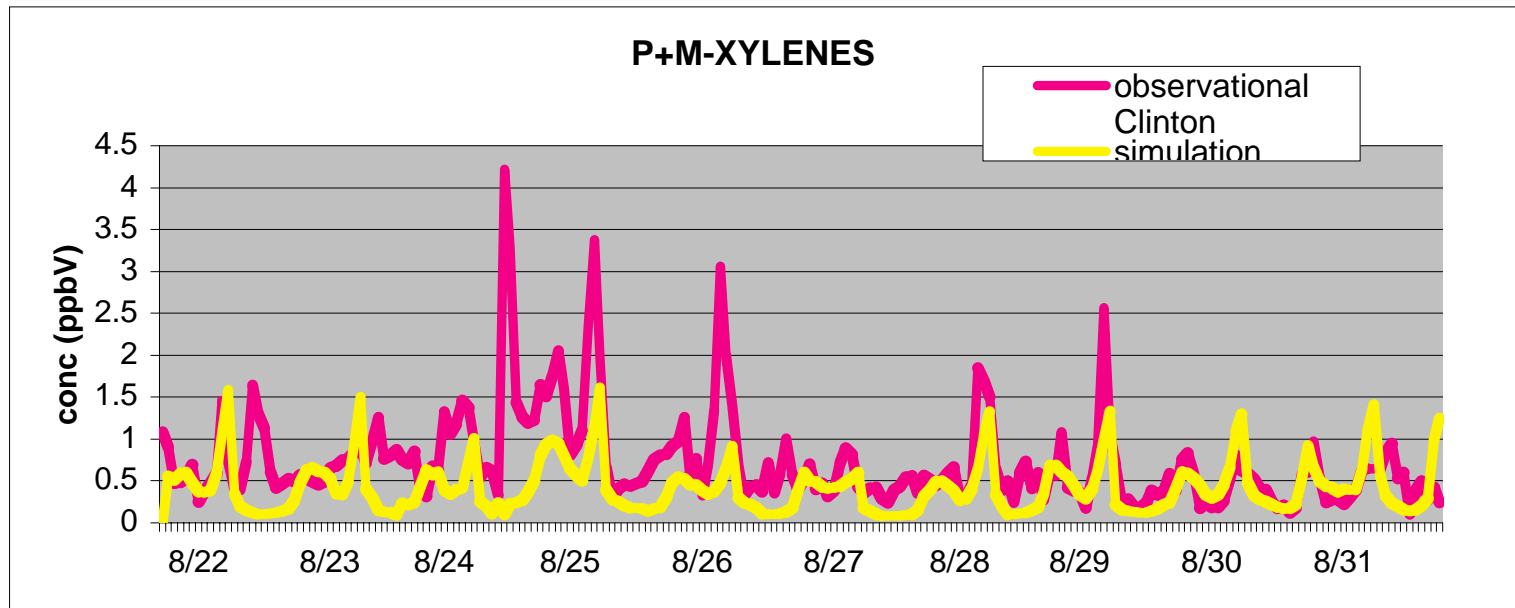
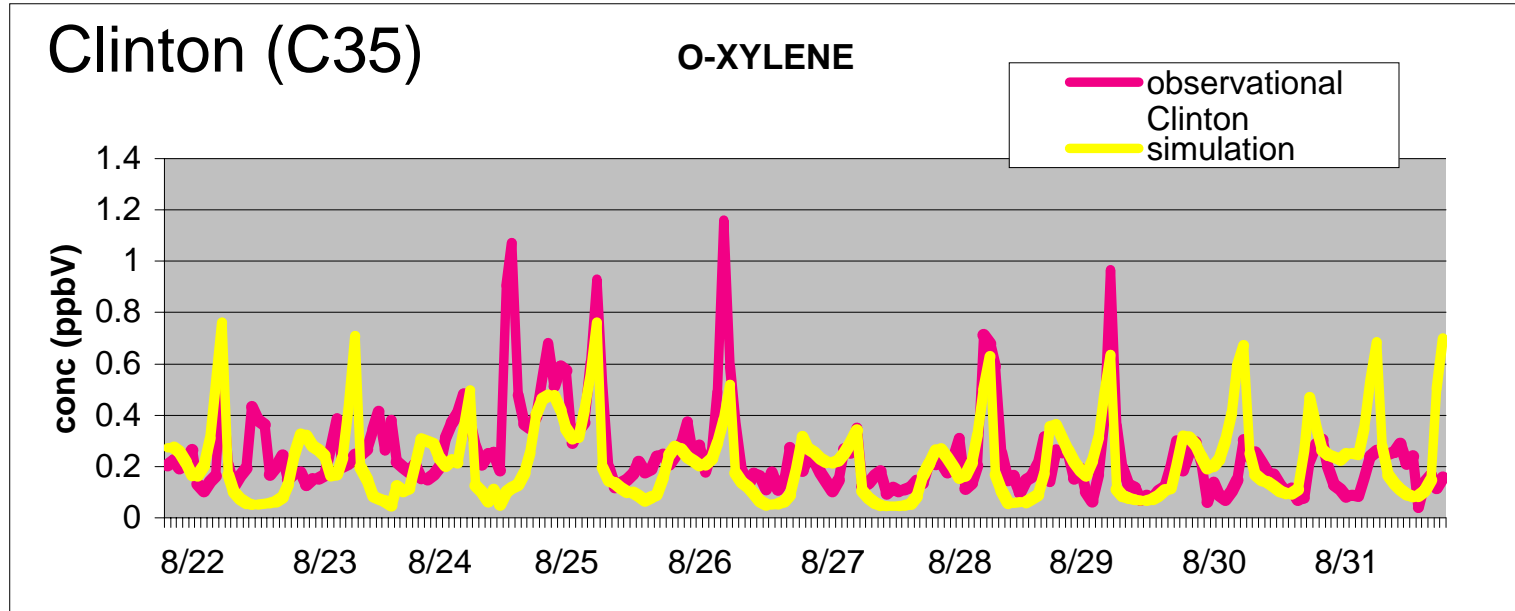
- Overall, ETH in Q74 is much lower (ca. 50%) than ETH in X19.
- Still, both models over-predicted OBS.

AG Simulation

28-30 Sept 2004 HGB Episode: BaseA
Neighborhood Best 1 hr NO₂



UH Air Toxics Simulation (Regular EI)



Results: VOC, NO₂

- VOC
 - Q74 showed much lower ETH, OLE than X19 but still over-predicts.
 - UH expanded SAPRAC without imputation suggests small bias in aromatics at clinton monitor
- NO₂
 - Q74 showed lower NO₂ than X19 but still over-predicts.
 - Preliminary analysis suggests less bias in AG post 2000 runs

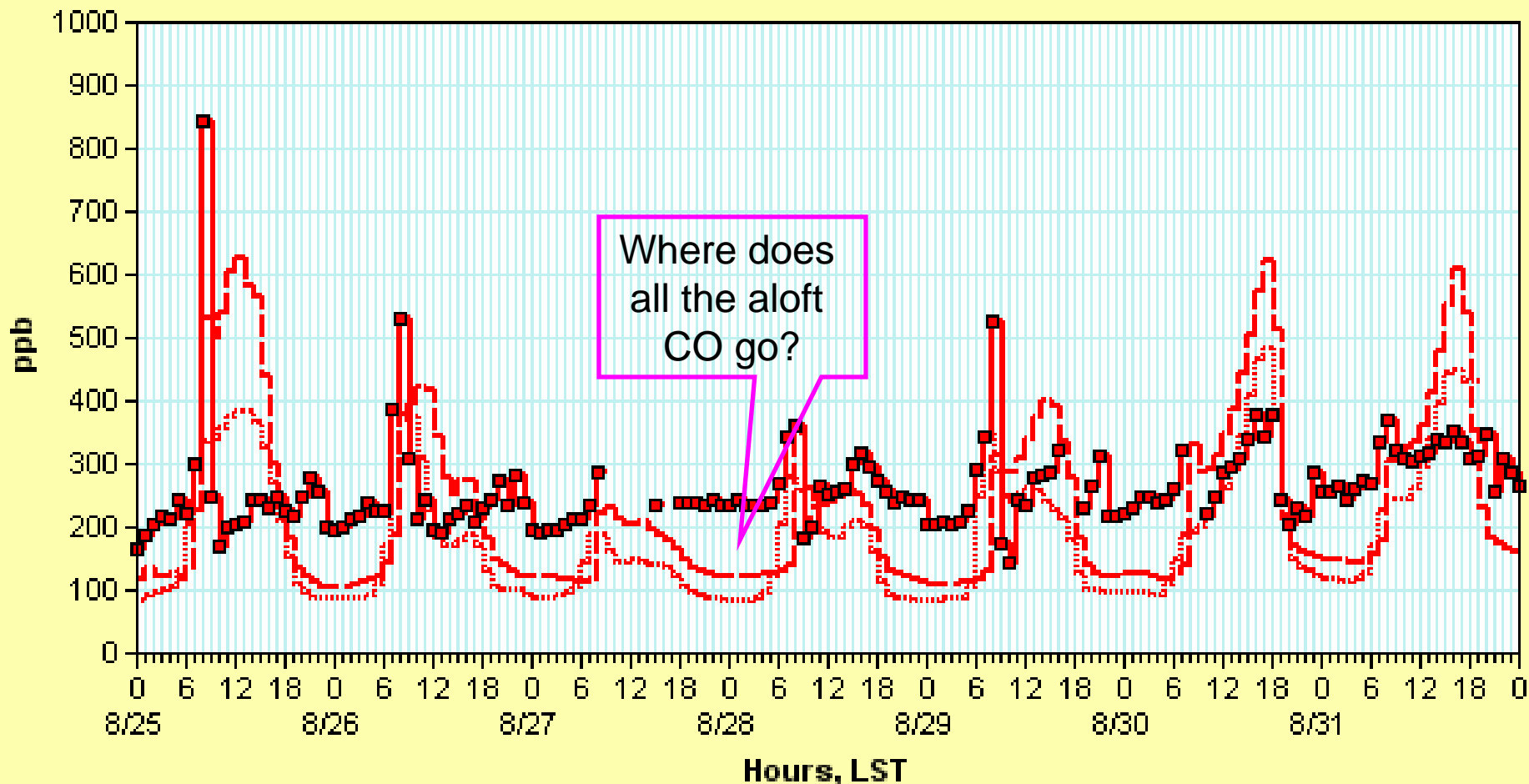
WLT, William's Tower (243m AGL), hourly, X002

CO

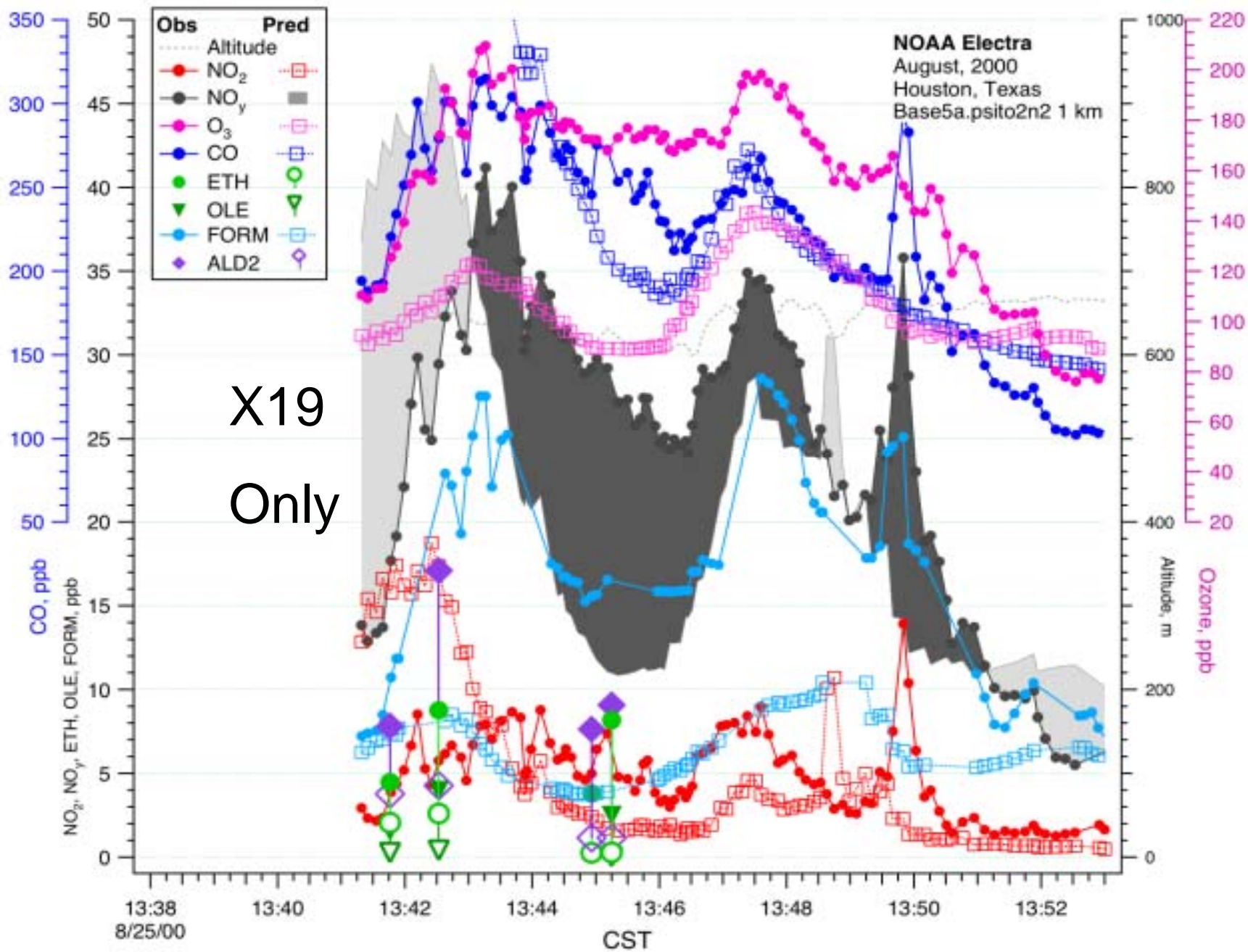
—■— CO

--- x19 in 4km by 1cell

..... q74 in 4km by 1cell



- X19 and Q74 showed large diurnal variation at 243 meters elevation while OBS did not.
 - Nighttime bias is nearly 100%
 - Q74 showed lower day and night values



Results: CO

- In general, Q74 showed lower CO than X19 and it is closer to OBS where OBS are available.
- Both show problem with aloft CO at WILT
 - Daytime is often predicted too high; (mobile CO too high)?
 - Nighttime is often predicted too low (ca. 0.5)
 - The nighttime loss of CO may also indicate a loss of other daytime produced products such as formaldehyde, higher aldehydes and other “carry over” radical sources.

How are the Houston models performing?

Conclusions

- UH MM5 produces a different, but acceptable realization of the wind fields without GOES2 adjustments.
- This met with TCEQ PSIT02N2 produces lower peak NO and lower NO₂, and sometimes slightly more O₃
- TCEQ and UH model incorrectly predict CO, especially at night aloft. Suggest that model cleans itself out too fast and loses “radical sources” necessary for the next day to be adequately reactive.
- Aloft NOAA aircraft obs vs data show poor prediction of HCHO, CO, NO_x.
- TCEQ model predicts 2x to 5x more biogenic ISOP than observed. UH does better in some locations but not others.

How are the Houston models performing?

Conclusions

- Post-2000 AG simulations show essentially no mean NO₂ bias. Caused by different mobile sources EI or met?
- UH Air toxics simulation with “regular” EI and UH met show very good agreement with obs. Suggesting that no imputation for aromatics is needed at clinton for this episode.
- Changing to current “best science” improves the model, but does not “fix” it so that model is still biased and may not respond correctly to VOC or NOx controls.
- Need to investigate how to ‘fix’ radical sources in ALL models. This is as much a met problem as a VOC EI problem, and a Mobile EI problem.

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How Should We Design the TexAQS II-2006 Intensive?

- Emissions to the atmosphere
 - More speciated VOC concentrations (HRVOC, air toxics, OVOC)
 - SAPRAC mechanism is needed
 - Upset emission database
- Meteorology
 - Higher spatial resolution research grade CO network
 - Wind field measurements aloft

How Should We Design the TexAQS II-2006 Intensive?

- Chemical Reactions
 - Jochen Stutz radical measurements
 - Daum/Kleinman obs. based “ozone productivity” as a function of NO_x
 - Process rates model and observed, aloft and ground
 - Nighttime measurements

Future work

- Need vertical concentration gradients
 - Aerodyne van and aircraft
- Need to improve Process Analysis integration with models to show the relative strengths of radical initiation and termination in all models
- Q74 sensitivity runs with added “radical sources” from both NO_x and organic sources need to be done to determine how much more reactive the system will be.
- More aloft wind and pollutant concentration analysis needs to be performed.