

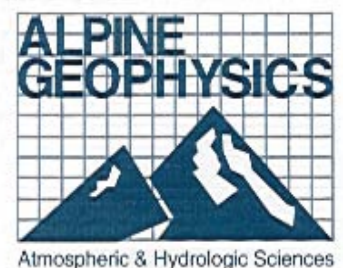
Integration of Multi-platform Modeling Analysis and 2006 Field Measurements to Explain Ozone Sensitivities in Houston And SE Texas

Harvey Jeffries and William Vizuete, UNC-CH
Tom Tesche, Alpine Geophysics

February 21, 2008



Presented to
TERC Science Advisory Committee



The UNC Team And Friends

Team
responsibilities
Sources of
information

HARC Research Team

UNC-CH

Harvey Jeffries - CO-PI
William Vizuete- CO-PI
Four Graduate Students

AQMs evaluation
Cross AQMs evaluation
sensitivity testing
pyPASS, pyPA, pyCSSOM

Alpine Geophysics

Tom Tesche
Dennis McNally
James Wilkinson
Cythia Loomis

MM5 sensitivity testing
μMM5 implementation
SMOKE high resolution EI
AQM sensitivity testing
OSAT-type testing



Collaborators

EPA

Alice Gilliland - ORD
Jonathan Pleim - ORD
Rob Pinder - ORD
Golam Sarwar - OAQPS

Share CMAQ code and files. Share students.
port PA to EPA; ACM2 applications; CB05 chemistry

Texas A&M

John Nielsen-Gammon

MM5 and WRF files. Test Chemistry Impacts.

UT-Austin

David Allen
Elena McDonald-Buller

Biogenics EI files. Test Chemistry Impacts.

Univ Houston

Daewon Byun

MM5 and EI files. Test Chemistry Impacts.

8-Hour Coalition Group

HRM Site Data

Steven Smith/ Walt Crow

SMOKE Emissions

8-H Group Requests to TCEQ



TCEQ AQ Model Team

Any MM5/AQM and EI
Files Posted for any
episode

episode
Files Posted for any
Any MM5/AQM and EI
TCEQ AQ Model Team

8-H Group Requests to TCEQ
SMOKE Emissions
Steven Smith/ Walt Crow
HRM Site Data
8-Hour Coalition Group

Wish to remind you of the type of work the UNC “core” team does.

- We are not AQ Modelers, per se: we are model analysts and model diagnosis folks.
 - ▶ We have learned that it is dangerous to accept a model’s prediction (even a very good one) at face value.
 - ▶ Using tools and methods we have developed over years, instead we figure out how the models predicted what they predicted. That is, we re-cast the model’s predictions of concentration fields into the more abstract level of “process parameters”, common to all AQMs and we examine if the magnitudes and competition, and compensation among these make sense given what we know about the real world.
 - ▶ At this level, we can compare different model formulations, (eg CAMx vs CMAQ), different chemical mechanisms, different scenarios, and find meaningful explanations of the different outcomes (often involving complex feed back paths).
 - ▶ By understanding this, we can generate meaningful sensitivity cases and investigate how the model responds, and by illuminating why the model responds, we can generate testable hypotheses and determine what observations are suitable for discriminating among competing formulations or inputs in the models.

Investigation of Limited Radical Source Strength in the Houston Regulatory Ozone Model

TERC Science Advisory Committee Meeting
HARC, The Woodlands, TX

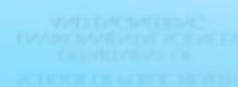
Harvey Jeffries¹ and William Vizuete

University of North Carolina



November 9, 2006

NOVEMBER 9, 2006



We reported on our Process Analysis/Sensitivity Study on Radical Limitations in the TCEQ SIP model, such that the mere addition of more HRVOC could not 'fix' the model to agree better with the world, but that a critical element (given the other conditions in the inputs) of a primary radical source was needed to have the model respond more like the real world. This has consequences for testing potential policies.

Based on H60 project

Primary HCHO Most Effective at Producing More O₃

Availability of VOC or NO_x is not controlling O₃

- ▶ the base model only reacts 33% of the available VOC and this limits the amount of O₃ that can be produced
- ▶ ·OH will react with available NO₂ to terminate and will react with available CO to propagate ·OH but not create any new ·OH; this limits the amount of ·OH available to react with VOC
- ▶ in the absence of reaction with ·OH, horizontal transport disperses much of the emitted VOC unreacted

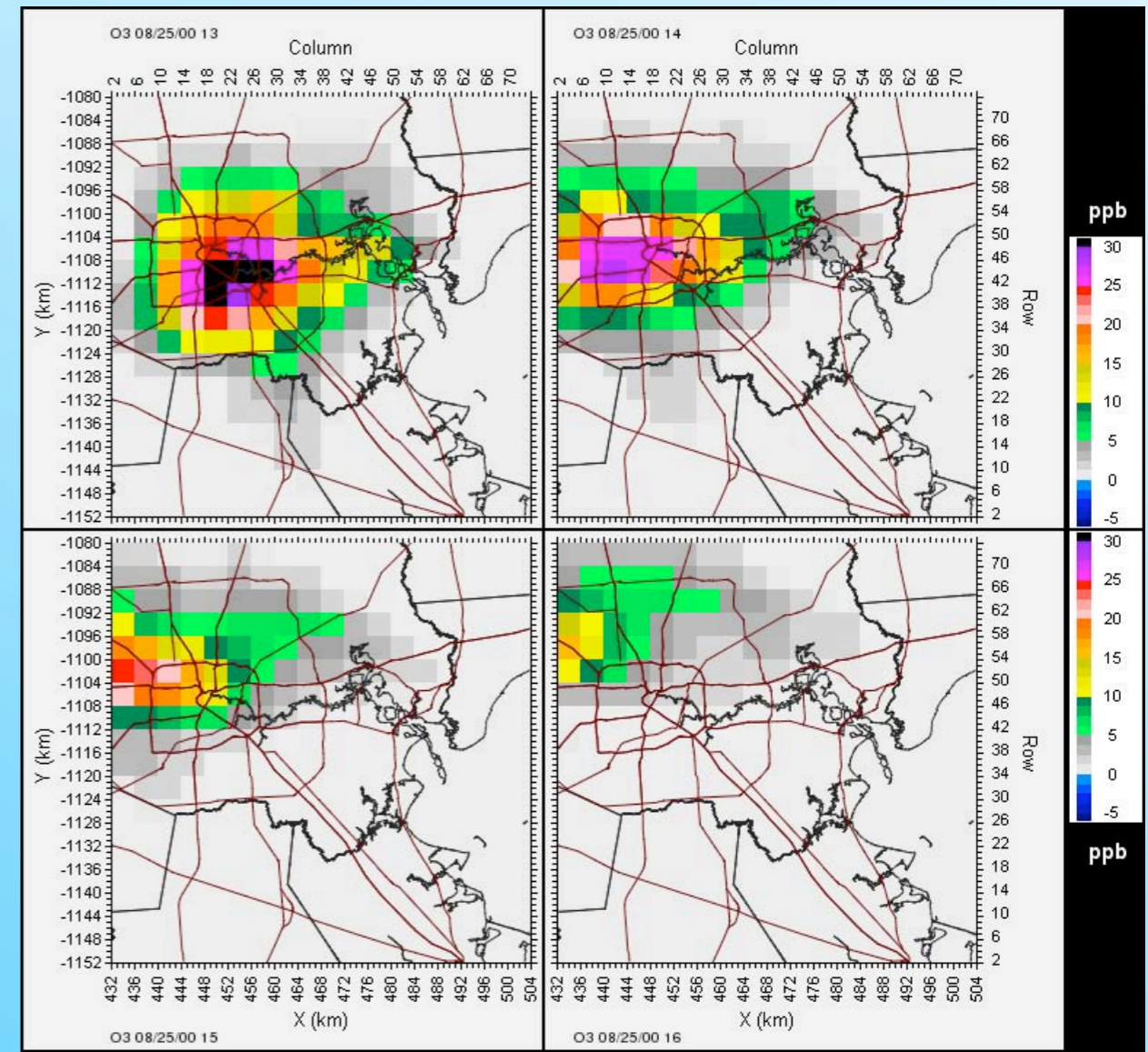
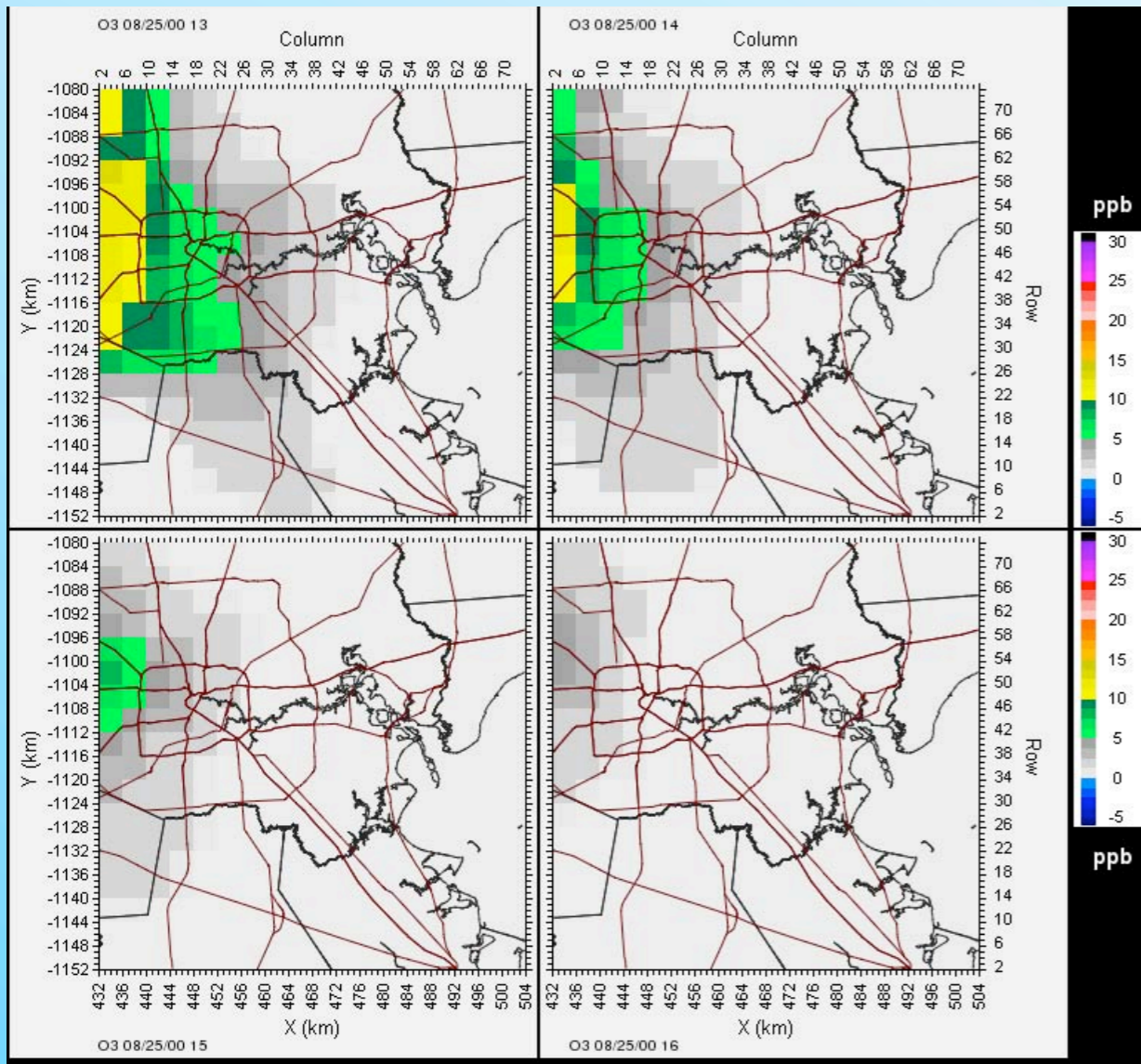
Adding more HRVOC does not help

- ▶ the HRVOC must react with existing ·OH to produce products that will contribute new ·OH
- ▶ the delay causes peak O₃ to be lower and to produce less new ·OH via O₃ + hν
- ▶ primary sources of HCHO, either from point sources or from low-level distributed sources are very effective in creating more O₃: a gain factor of about 12 for each ppb of primary HCHO that photolyzes.

- ▶ distributed sources are very effective in creating more O₃: a gain factor of about 12 for each ppb of primary HCHO that photolyzes.
- ▶ primary sources of HCHO, either from point sources or from low-level distributed sources are very effective in creating more O₃: a gain factor of about 12 for each ppb of primary HCHO that photolyzes.

Based on H60 project

August 25, 2000, 13-14 CST



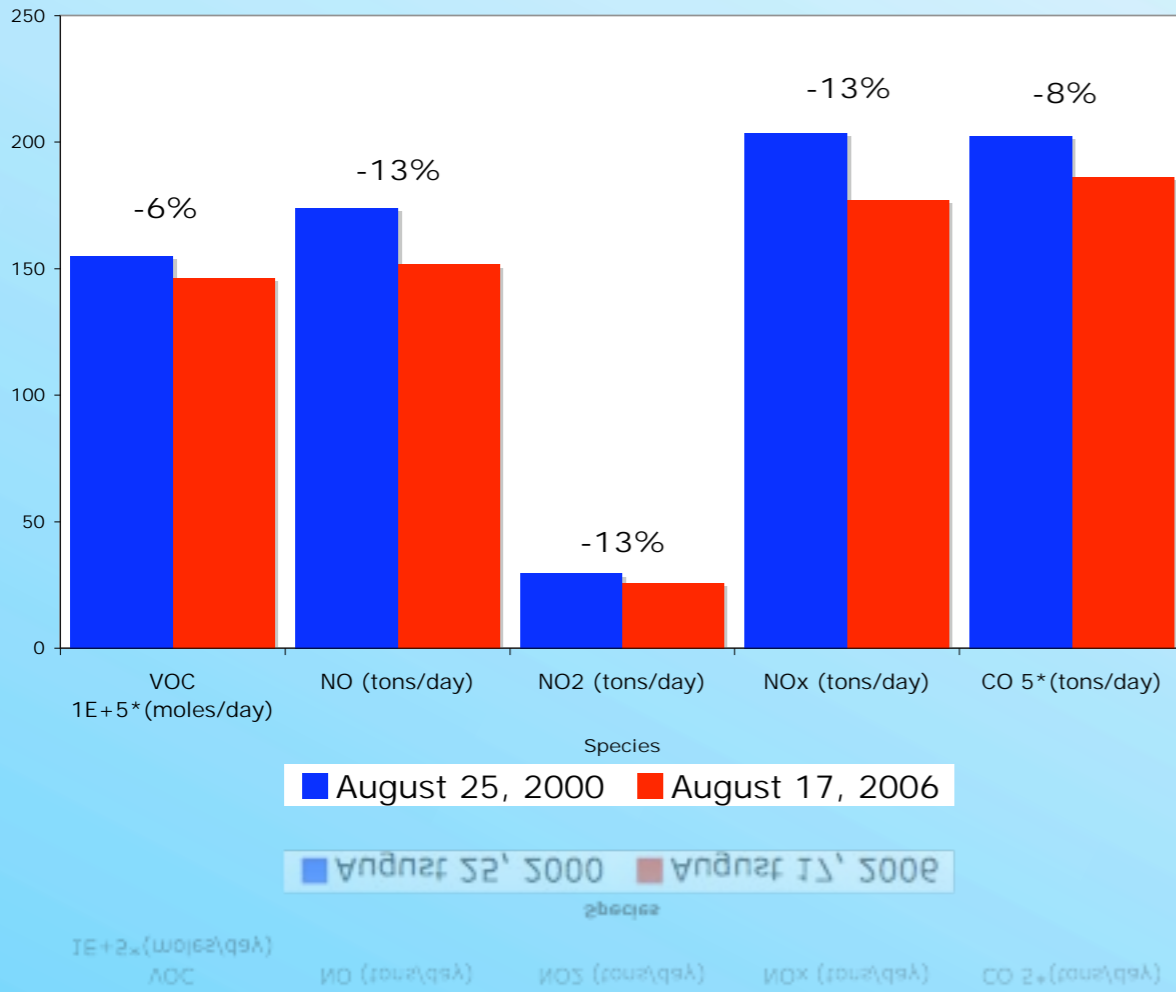
Above:
Change in O₃ from adding 2.8 t/d ETH

Right:
Change in O₃ from adding 1.3 t/d FORM at flares



Based on H87 project

August 25, 2000, CHOU, CAMx
August 17, 2006, CHOU, CMAQ

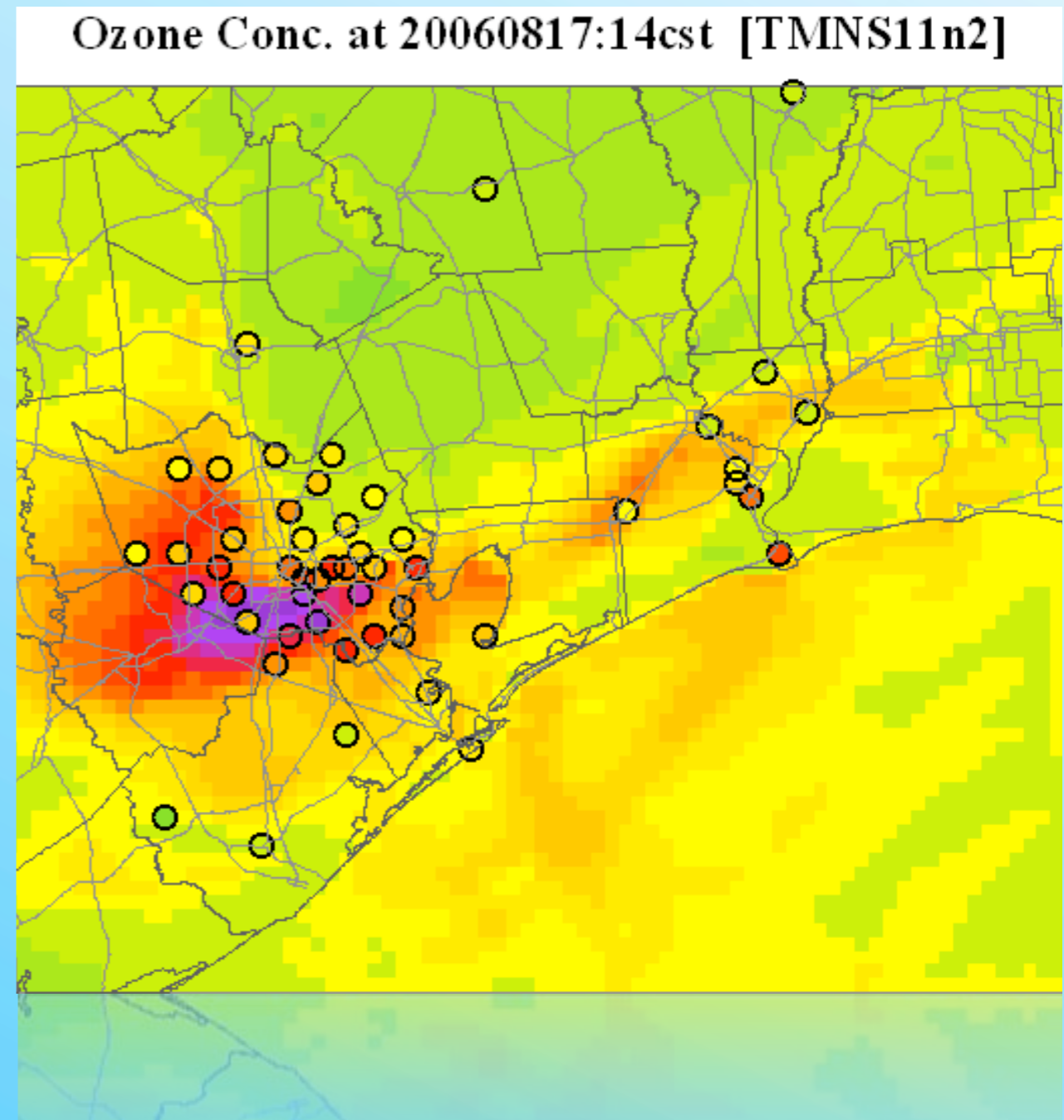


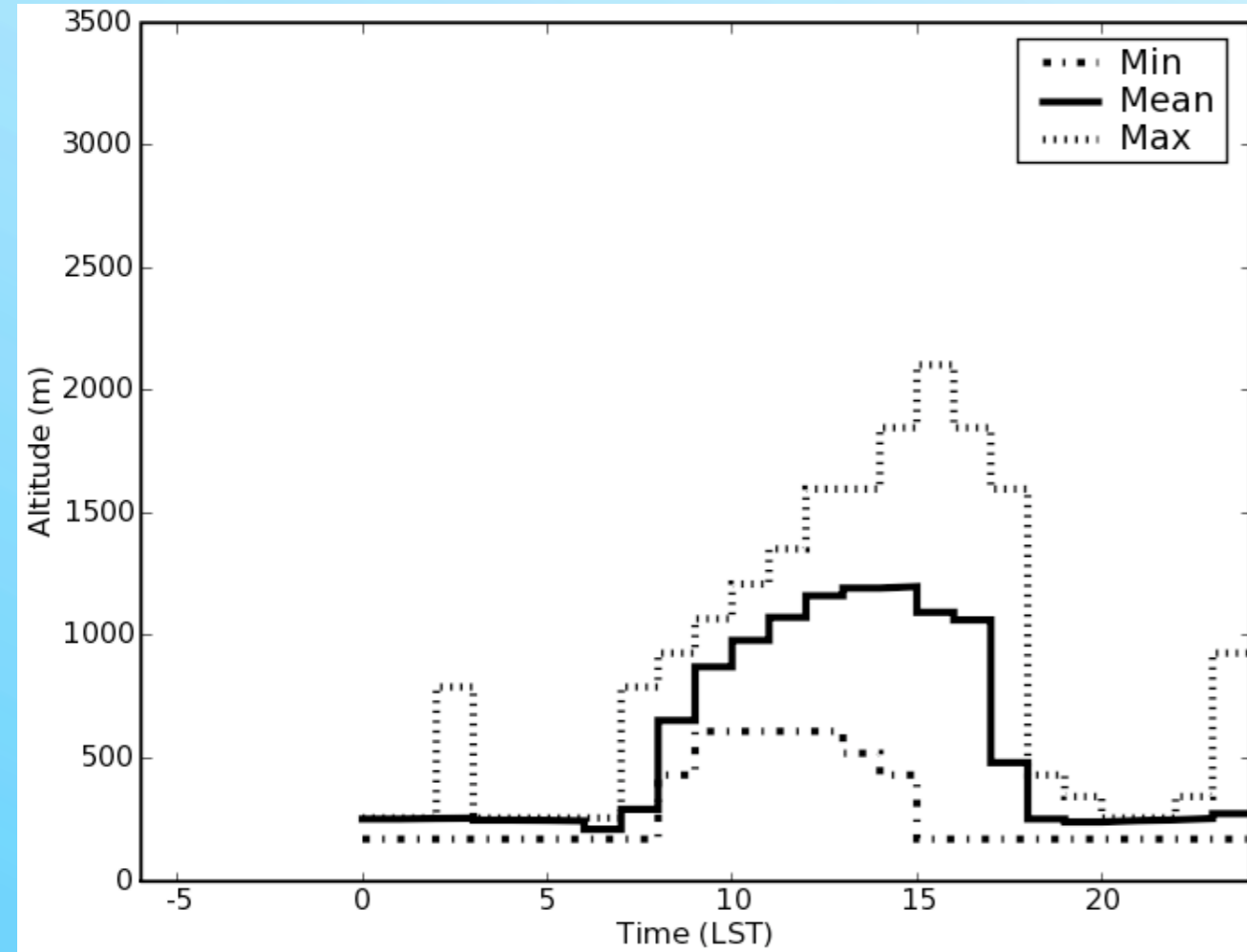
Above:
Change in Emissions from 2000 to 2006 in
CHOU

Right:
O₃ predicted by CMAQ in 2006.

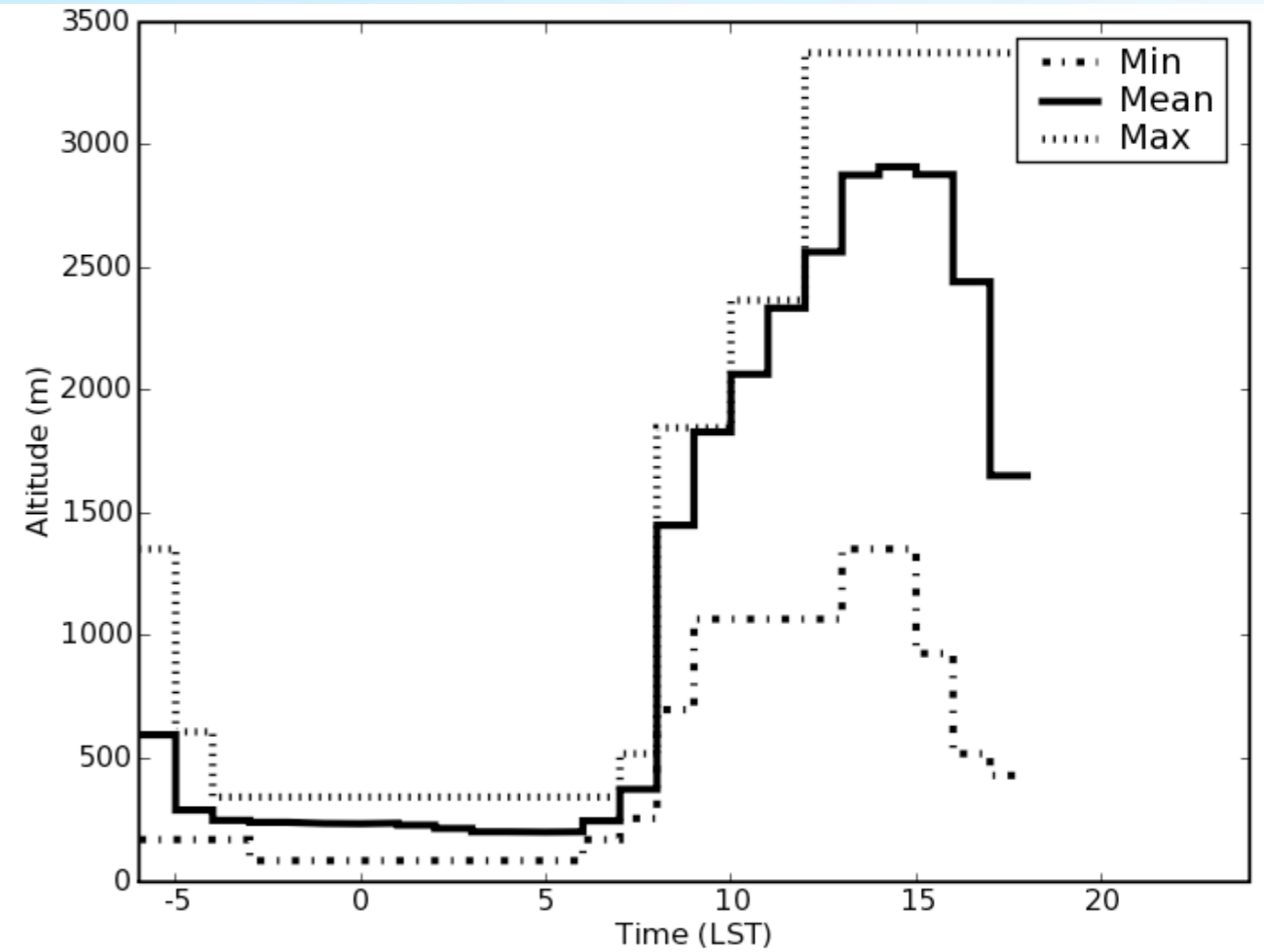
Same 'new OH', reacted more VOC, made 15 ppb
more O₃ than 2000 case.

NO_x-limited after 12 noon!



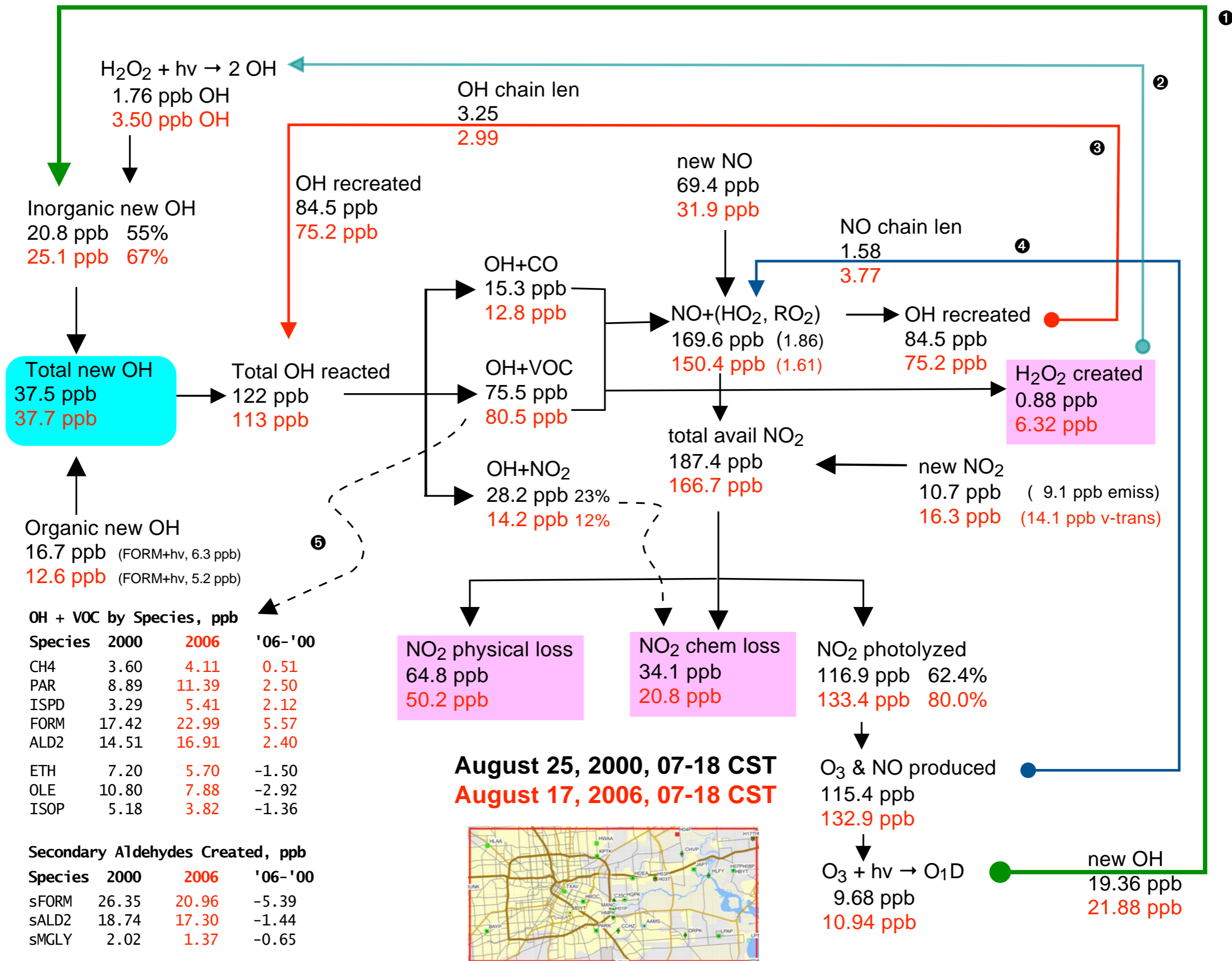


8/25/2000 CAMx

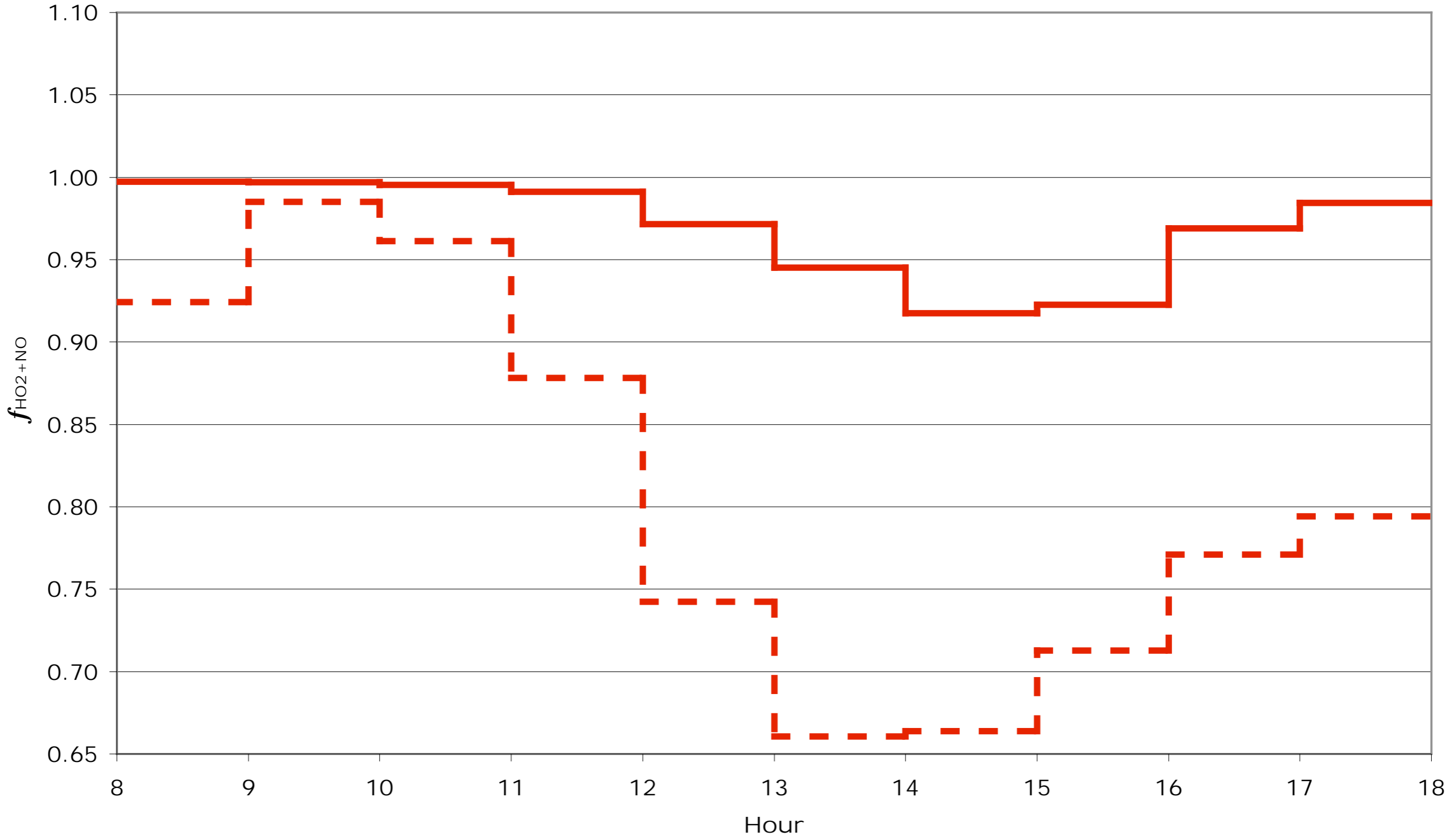
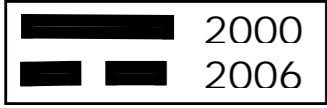


8/17/2006 CMAQ

It is the meteorology!



Fraction of HO2 reacts with NO



Which is it?

- If this scenario and met inputs describes post-2000 Houston, then the SIP control strategies have it backwards.
- If Aug. 2006 was unusual, then we have another one-off study that will not provide good long-term SIP support.
- Certainly other met and chemistry models with inputs derived by different approaches need to be applied to this scenario to see if this results holds up for this day and others.

Goals of new work-I

- These two examples illustrate the benefits of the model analysis work we do. They also illustrate the dangers of depending upon a single episode and a single model representation.
- We wish to further extend the types of analyses we have done to include:
 - ▶ Two different AQM formulations: CAMx and CMAQ (same met, same EI)
 - ▶ Open-source EI at multiple resolutions and the explicit representation of 'events' known not to be included in Special EI; also, variations on Biogenics EI.
 - ▶ Two different met approaches: MM5 (and WRF) and micro-MM5

Goals of new work-II

- Investigate Vertical Mixing representations
 - ▶ CAMx and CMAQ models versus VME data, lidar data, and available aircraft data
 - ▶ Vertical mixing algorithms - ACM2 being tested for MM5 and WRF by John N.-G. in collaboration with Jon Pleim, EPA. Jon will also work with UNC on the CMAQ chemistry model with ACM2.

Goals of new work-III

- LULC and Biogenics Emissions
 - ▶ As was seen in the UH modeling, applying SMOKE processing to TCEQ's biogenics resulted in a 21% increase in total VOCs in 4-k.
 - ▶ Dave Allen's Team at UT have been investigating effects of different LULC representations and data sources on isoprene predictions. Dr. McDonald-Buller will describe these studies later.
 - ▶ We will share met and emissions files with UT and evaluate alternative Biogenics Els.
 - ▶ PA will permit us to clarify the interaction between vertical mixing, emissions rates, and concentrations of isoprene.

Goals of new work-IV

- This year the UNC team is joined by a group of nationally recognized “real” AQ modelers (as opposed to us merely hacking on other’s files): Alpine Geophysics, Tom Tesche and staff.
 - ▶ Alpine Geophysics will bring to the Team a first-class program on emissions inventory processing and evaluation.
 - ▶ Alpine Geophysics will bring a long experience with MM5 modeling and preparing model ready files.

Expected Benefits Policy Relevance

- This research is heavily focused on providing immediate SIP modeling relevant information. It directly addresses the following needs in the TERC Strategic Research Plan sections:
 - ▶ 1.3, 1.5, 1.6, 1.7, 2.2, 2.3, 3.2, 5.3, 6.2, and 6.4