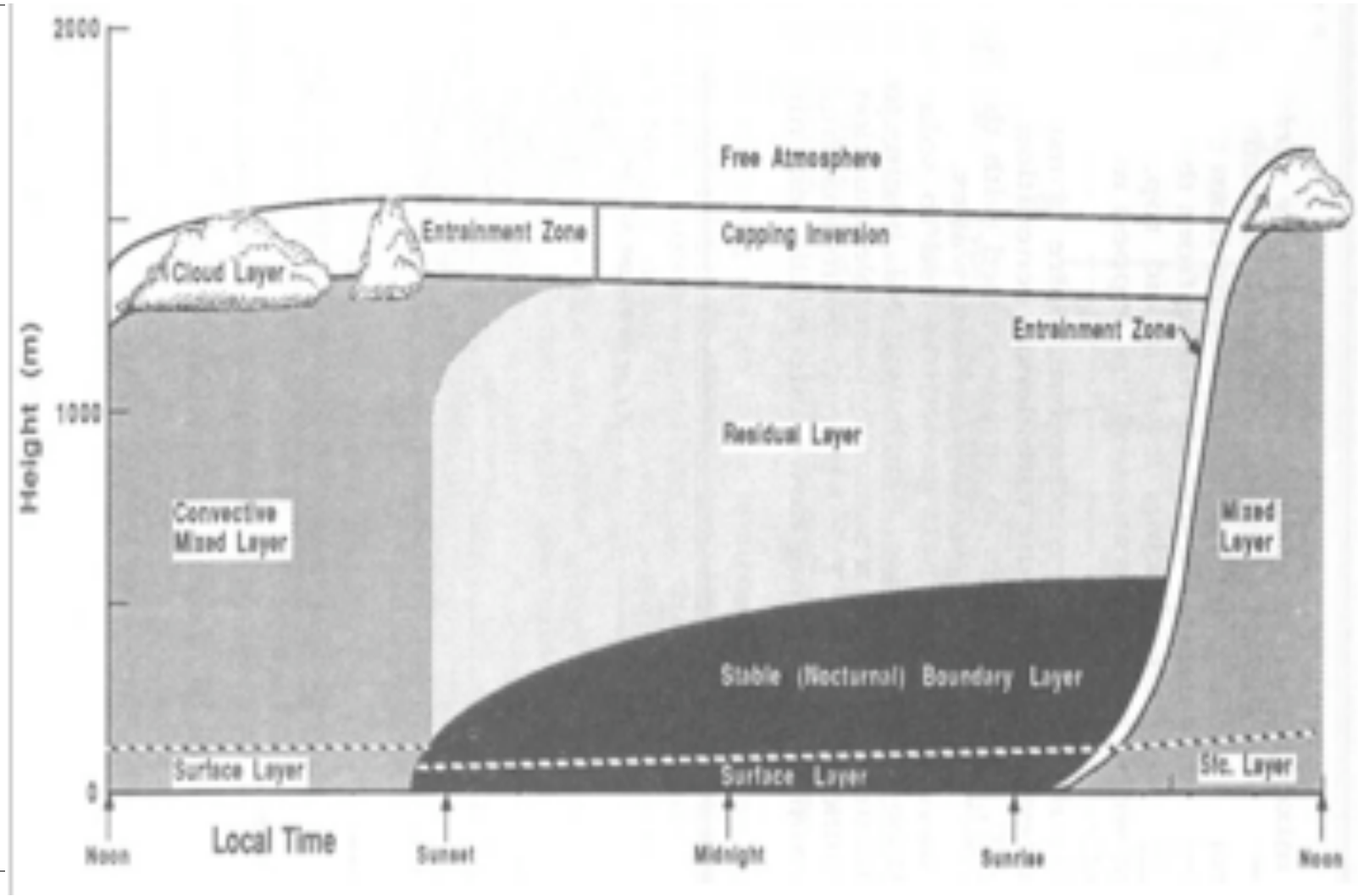
Process Analysis Techniques to investigate ozone production in regulatory simulations of Houston, TX

William Vizuete, Alejandro Valencia, Barron Henderson, Harvey Jeffries

2009 CMAS Conference
10/21/2009

Planetary Boundary Layer (PBL)



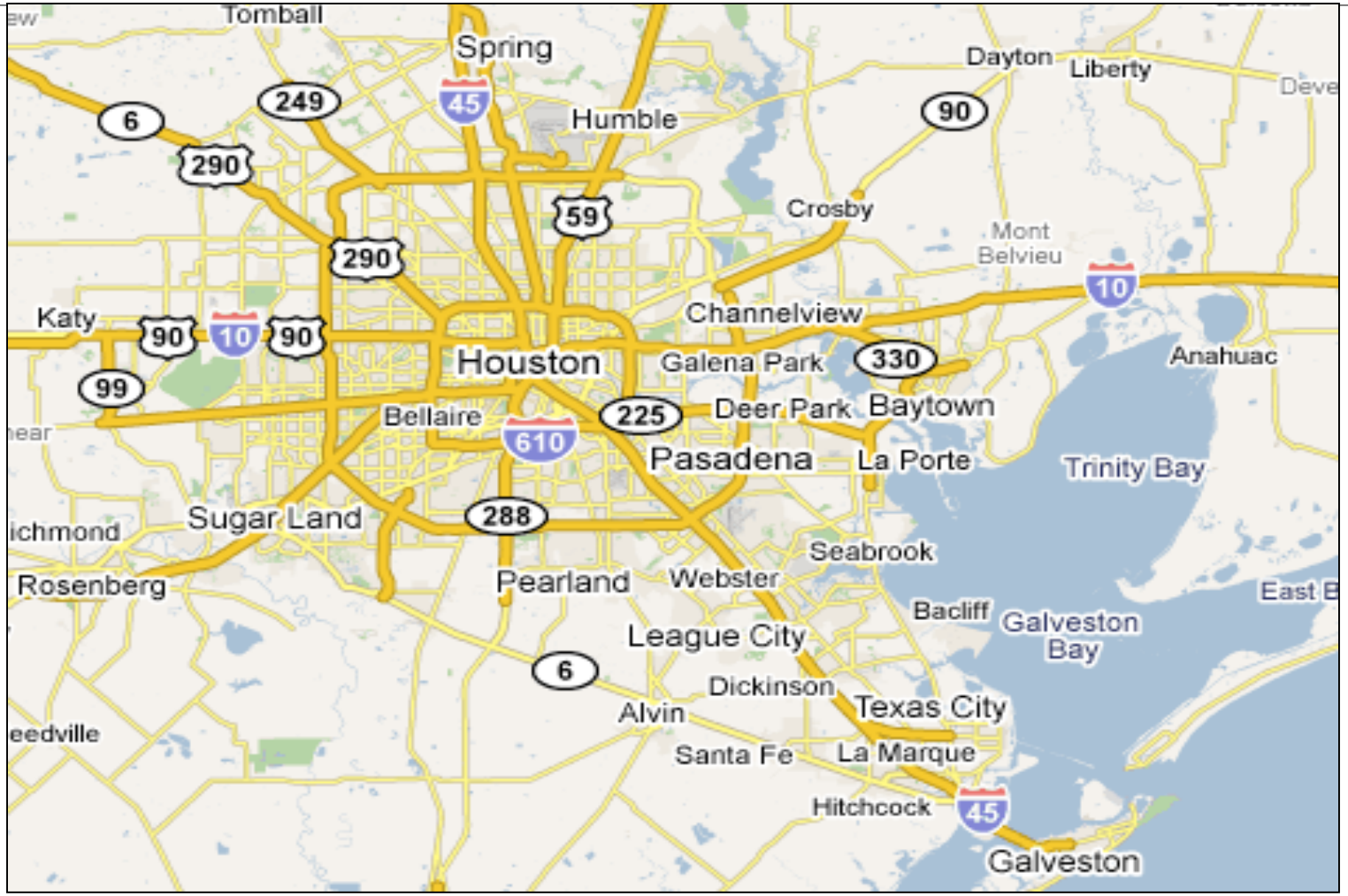
Planetary Boundary Layer (PBL)

How is model predicted O_3 sensitive to variability in the rate of rise of the Planetary Boundary Layer?

Outline

- Modeling Datasets
- Results
- Conclusions
- Future work

Houston,TX is a Non-attainment Area for 8-hr O3 (85 ppb)

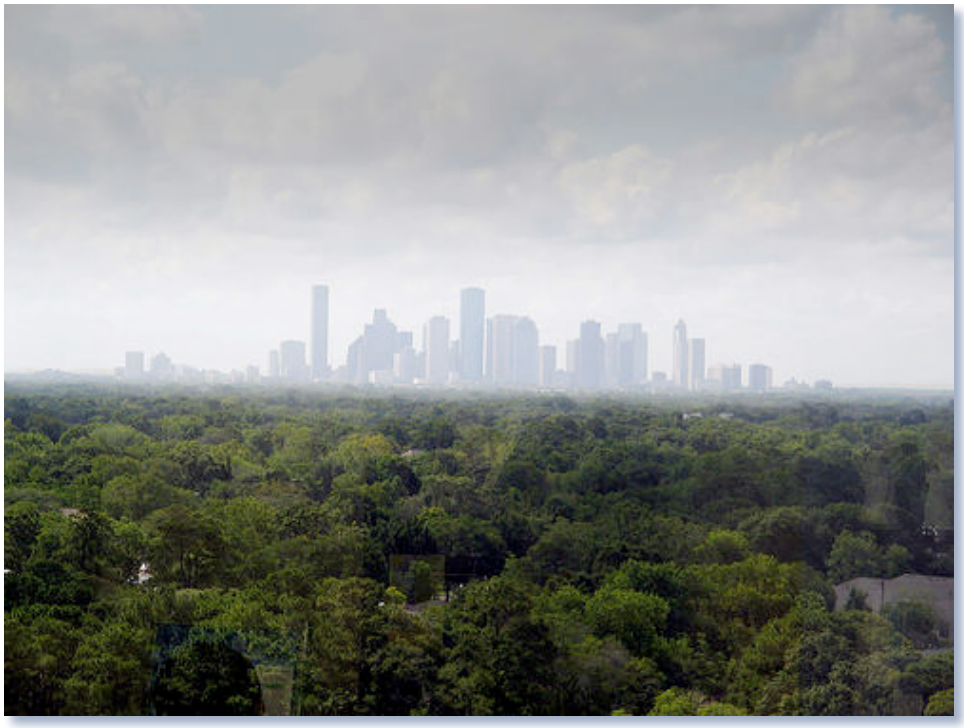


Modeling Dataset

- The Texas Commission of Environmental Quality (TCEQ)
- CAMx Air Quality Model Simulations
- 2000 Episode
  - 21 modeling days
- 2005/2006 Episodes
  - 120 modeling days

Outline

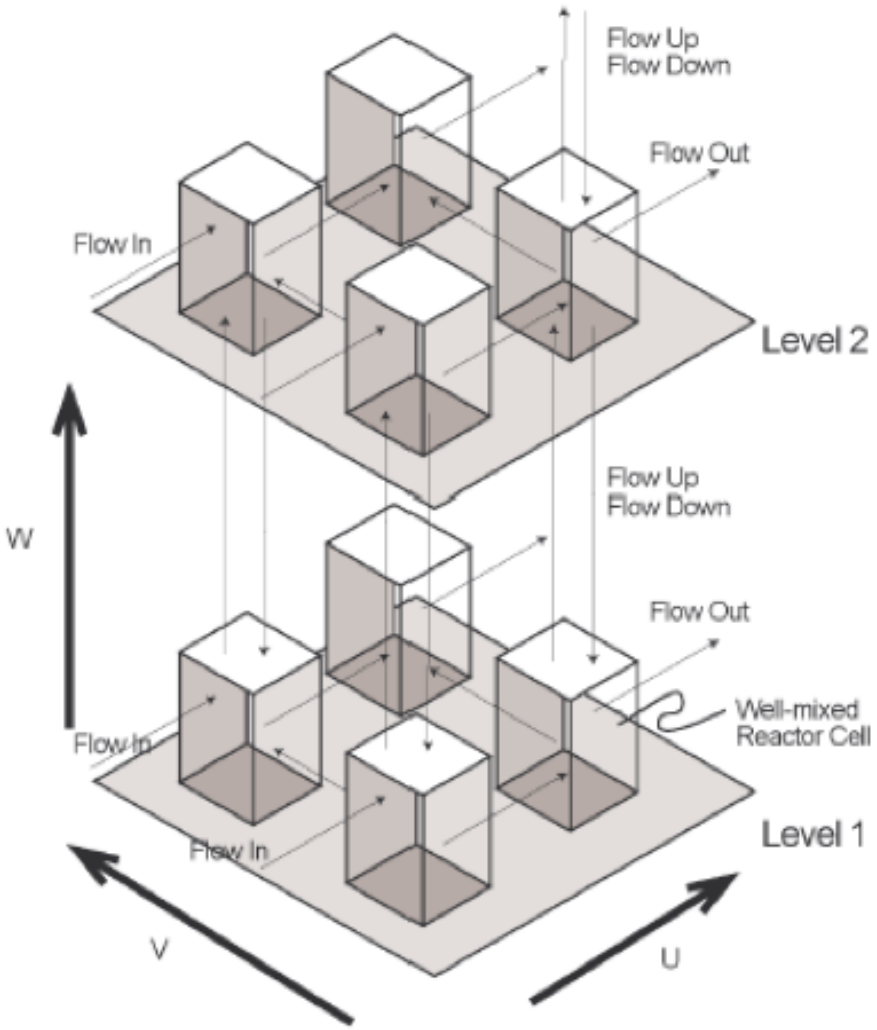
- Modeling Datasets
- Results
- Conclusions
- Future work



Simulated PBL

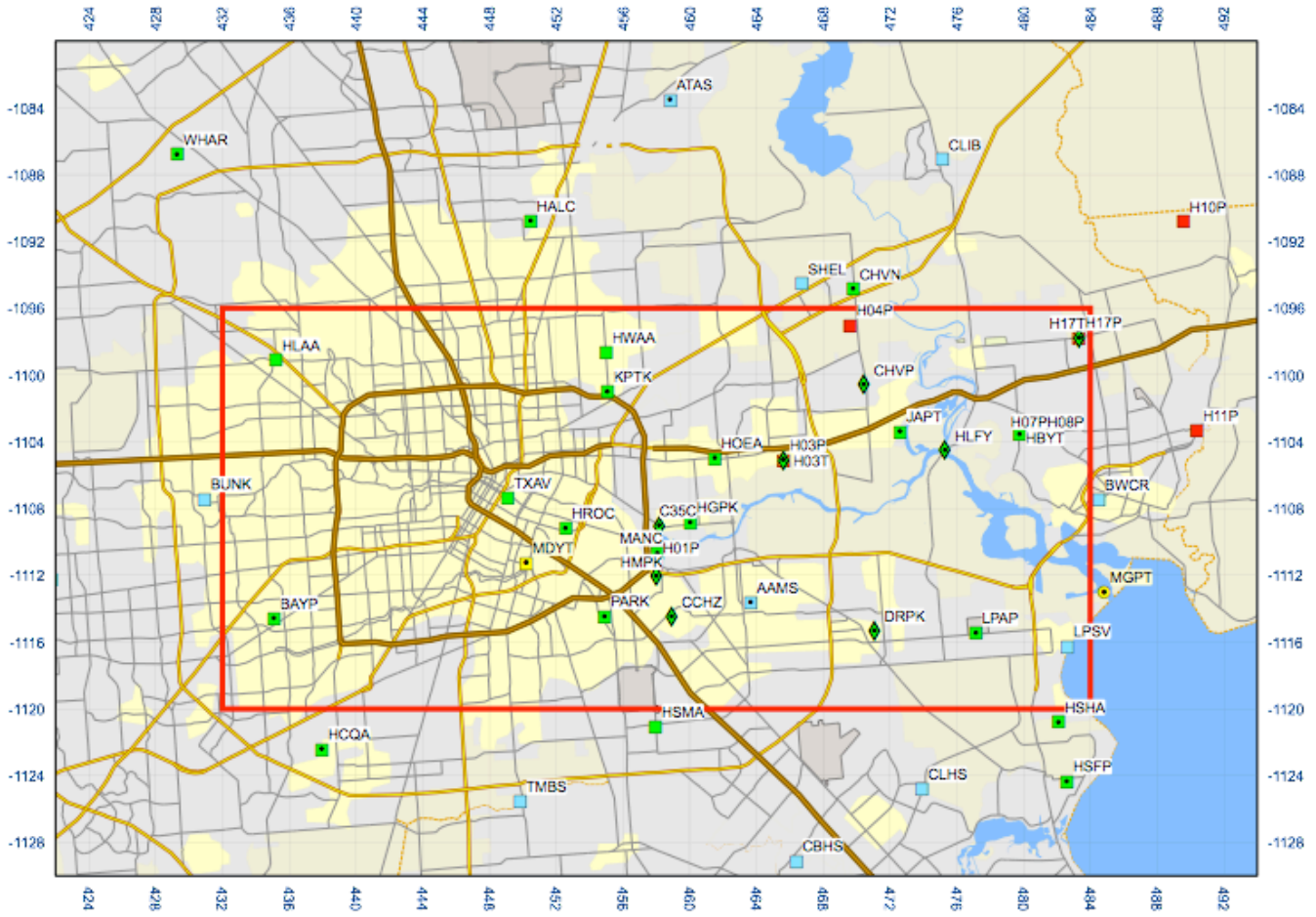
- CAMx: Found by extracting vertical mixing parameter (k_v) and calculating PBL

- Calculation made using same algorithm as ENVIRON's VERTAVG*

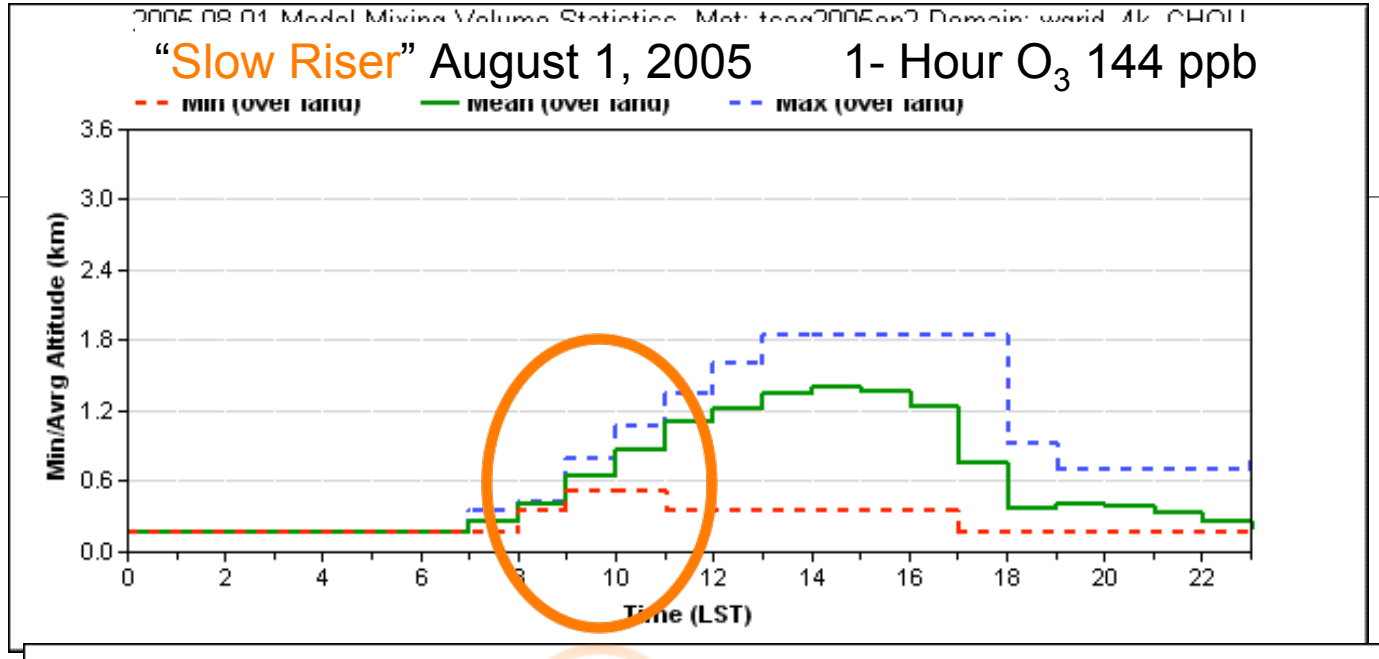


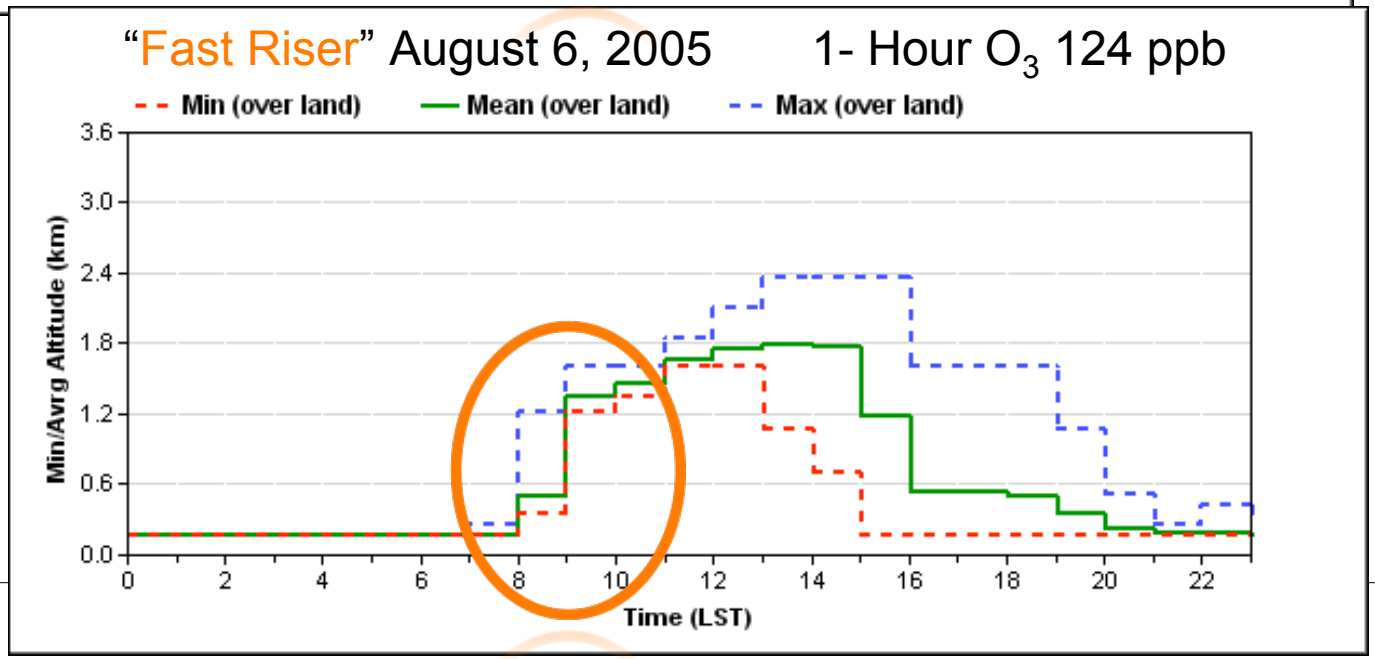
*Page 9-14 CAMx users guide

Focus on Central Houston

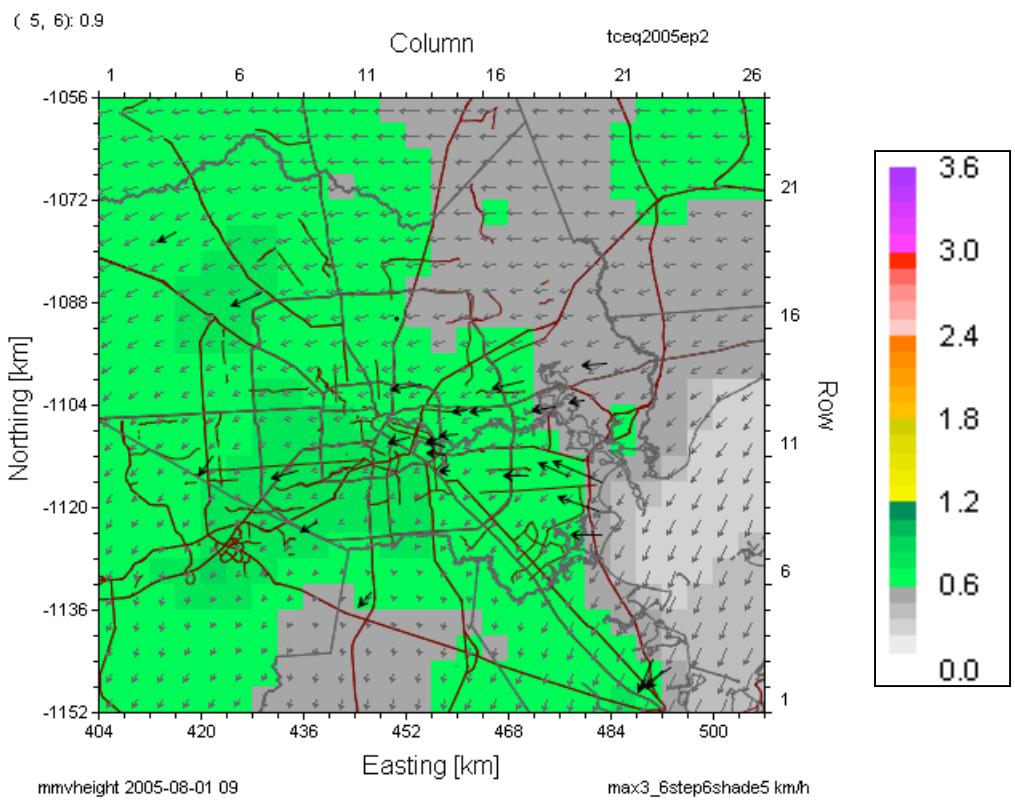


1,250 km^2

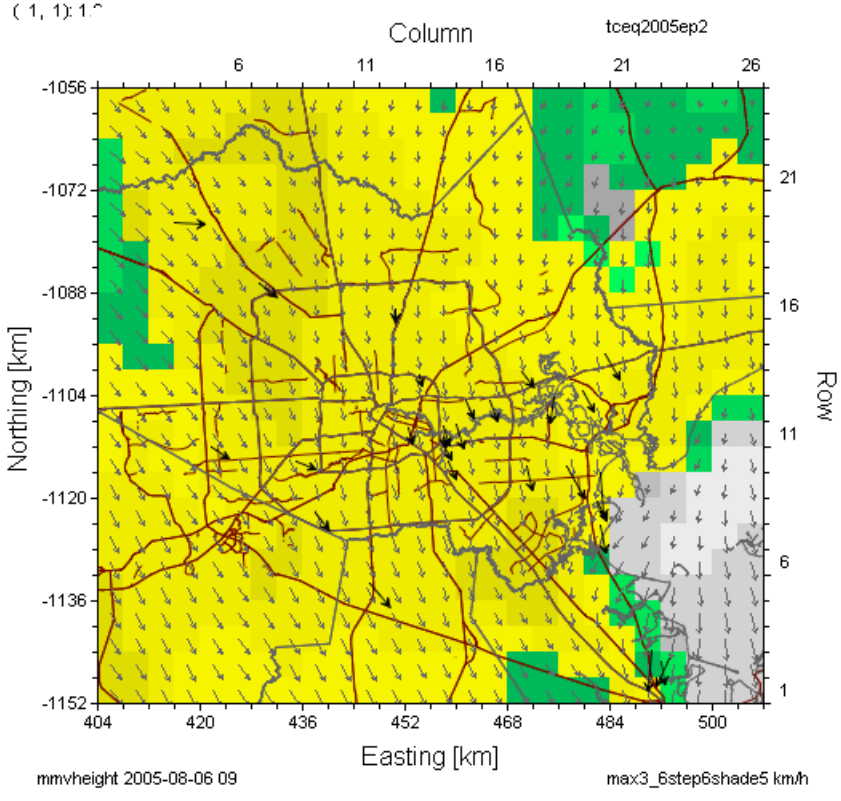

"Slow Riser" August 1, 2005 1- Hour O_3 144 ppb
Min (over land)
Mean (over land)
Max (over land)
Min/Avrg Altitude (km)
3.6
3.0
2.4
1.8
1.2
0.6
0.0
0
2
4
6
10
12
14
16
18
20
22
Time (LST)


"Fast Riser" August 6, 2005 1- Hour O_3 124 ppb
Min (over land)
Mean (over land)
Max (over land)
Min/Avrg Altitude (km)
3.6
3.0
2.4
1.8
1.2
0.6
0.0
0
2
4
6
8
10
12
14
16
18
20
22
Time (LST)

Fast Riser higher than Slow Riser



"Slow Riser" August 1, 2005 9 LST



"Fast Riser" August 6, 2005 9 LST

2 Distinct PBL Rises

- Slow Riser = PBL change less than 700 m/h

  between 6 to 11 LST

- Fast Riser = PBL change more than 700 m/h

  between 6 to 11 LST

Morning PBL Rise

- 2000:
  - Slow riser PBL on high ozone days
- 2005/2006
  - 63 modeling days with 8-hr Max O3 >85 ppb
  - 35% had a fast morning rise in PBL
- How were model processes changed?

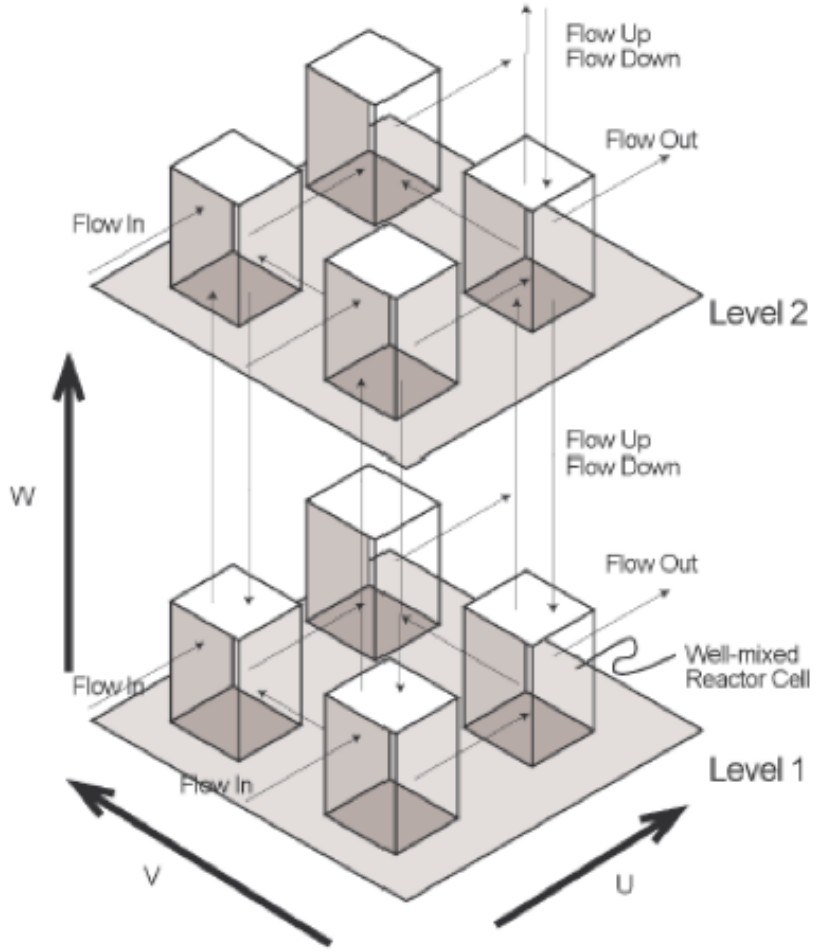
Process Analysis Results

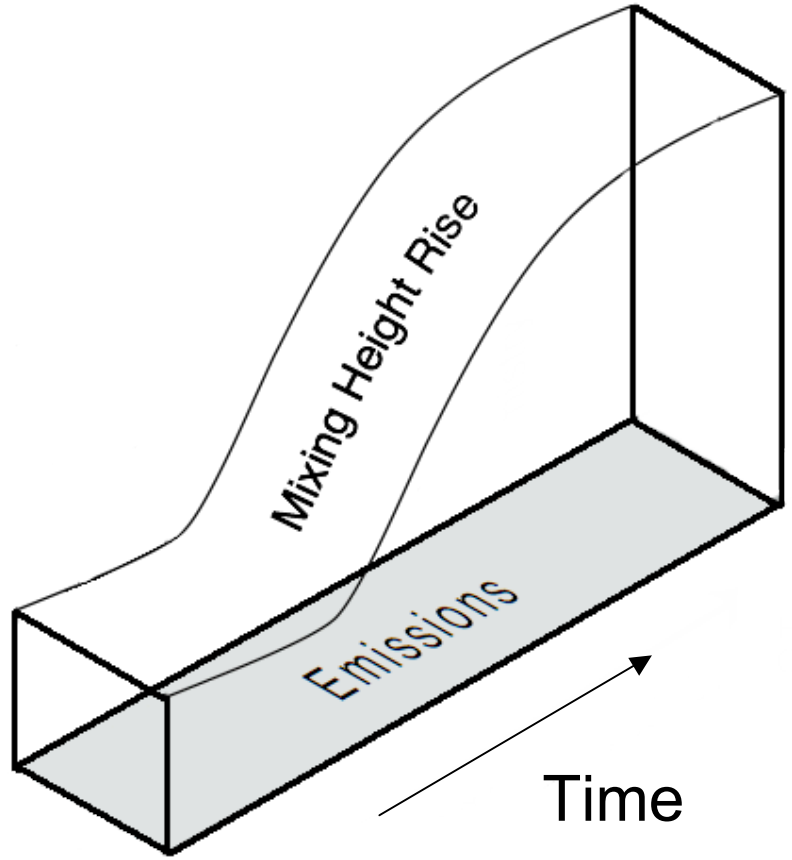
Model Evaluation and Analysis
Poster Session 10/20/2009
Python-based Environment for
Reaction Mechanisms (PERM)

Barron Henderson

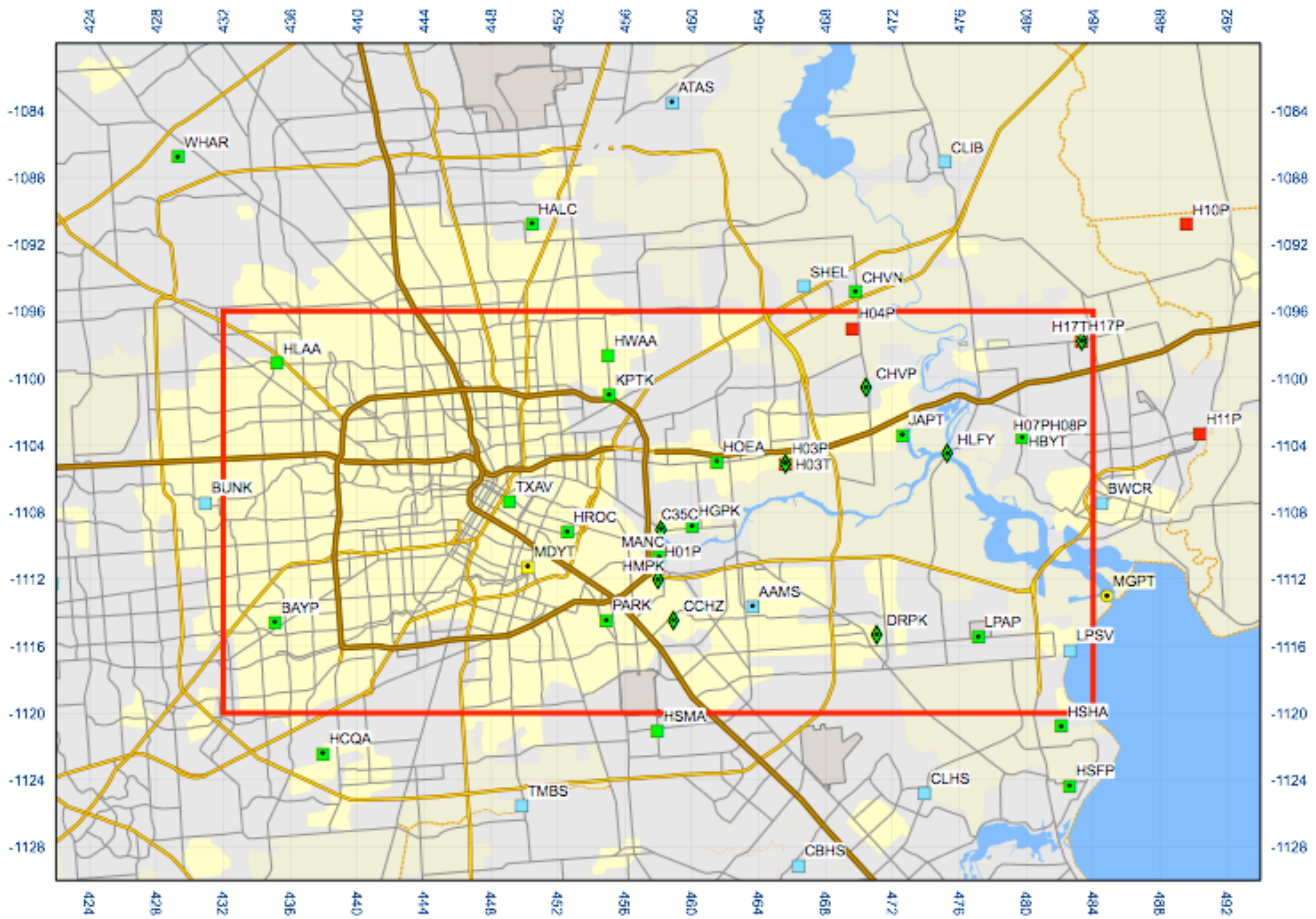
https://dawes.sph.unc.edu/trac/PERM

Process Analysis Aggregation: Vertical





Process Analysis Aggregation: Horizontal



1,250 km^2

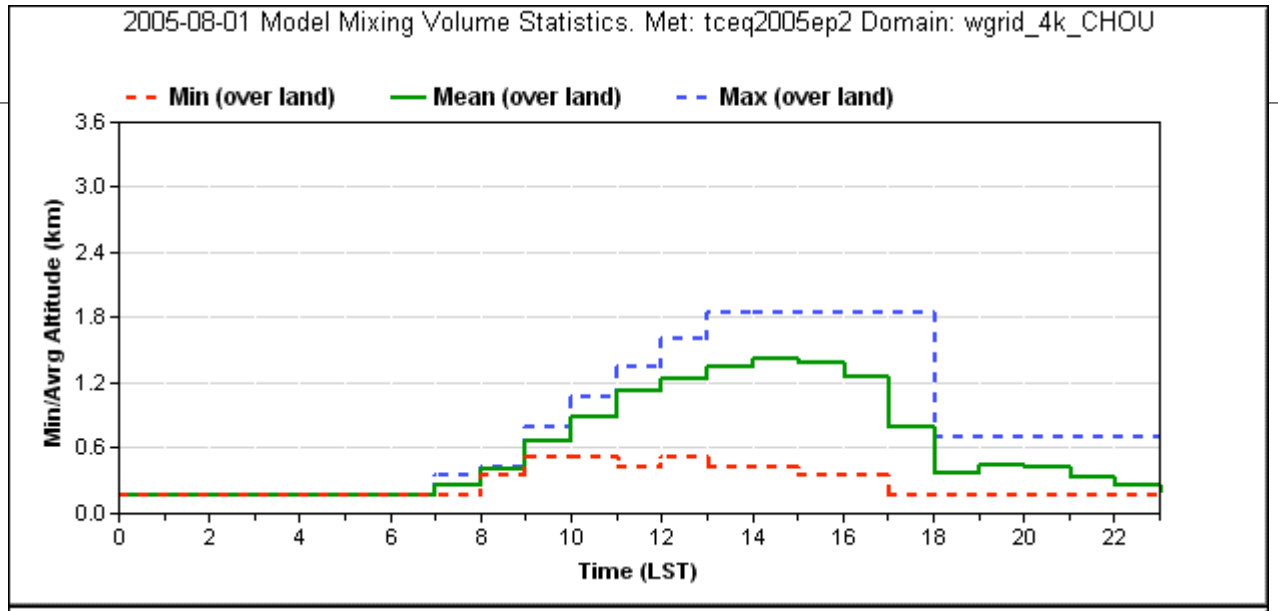
Model Experiment

2 New-modeled days

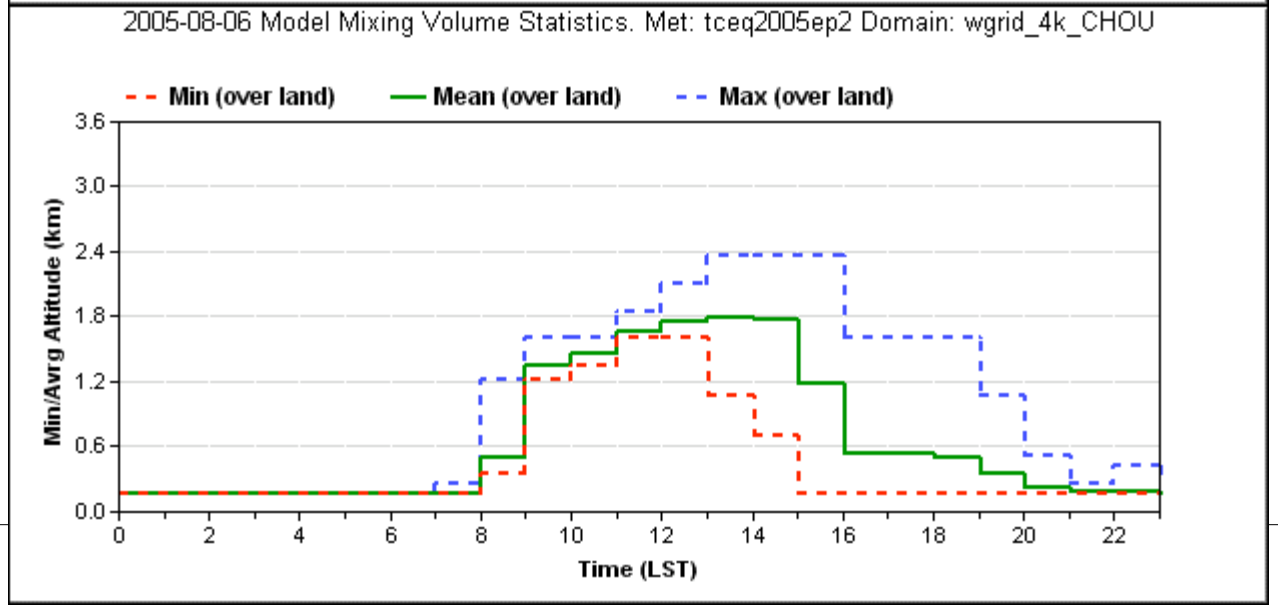
Emission Inventory	Meteorology (PBL Rise)
Weekday	Slow
Weekday	Fast

2 Meteorological Days

Slow Riser

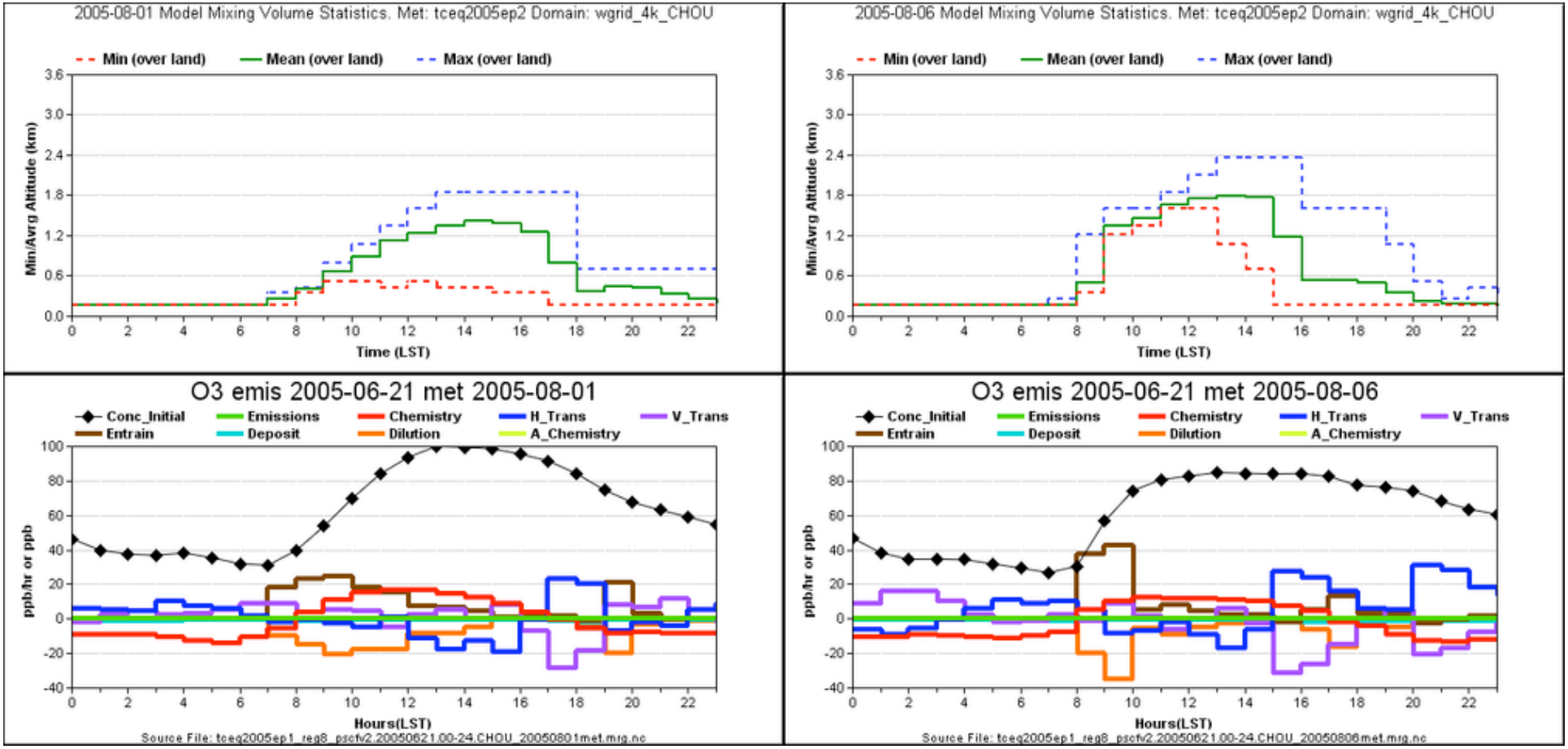


Fast Riser



Physical Processes : O3

06/21/05 Weekday

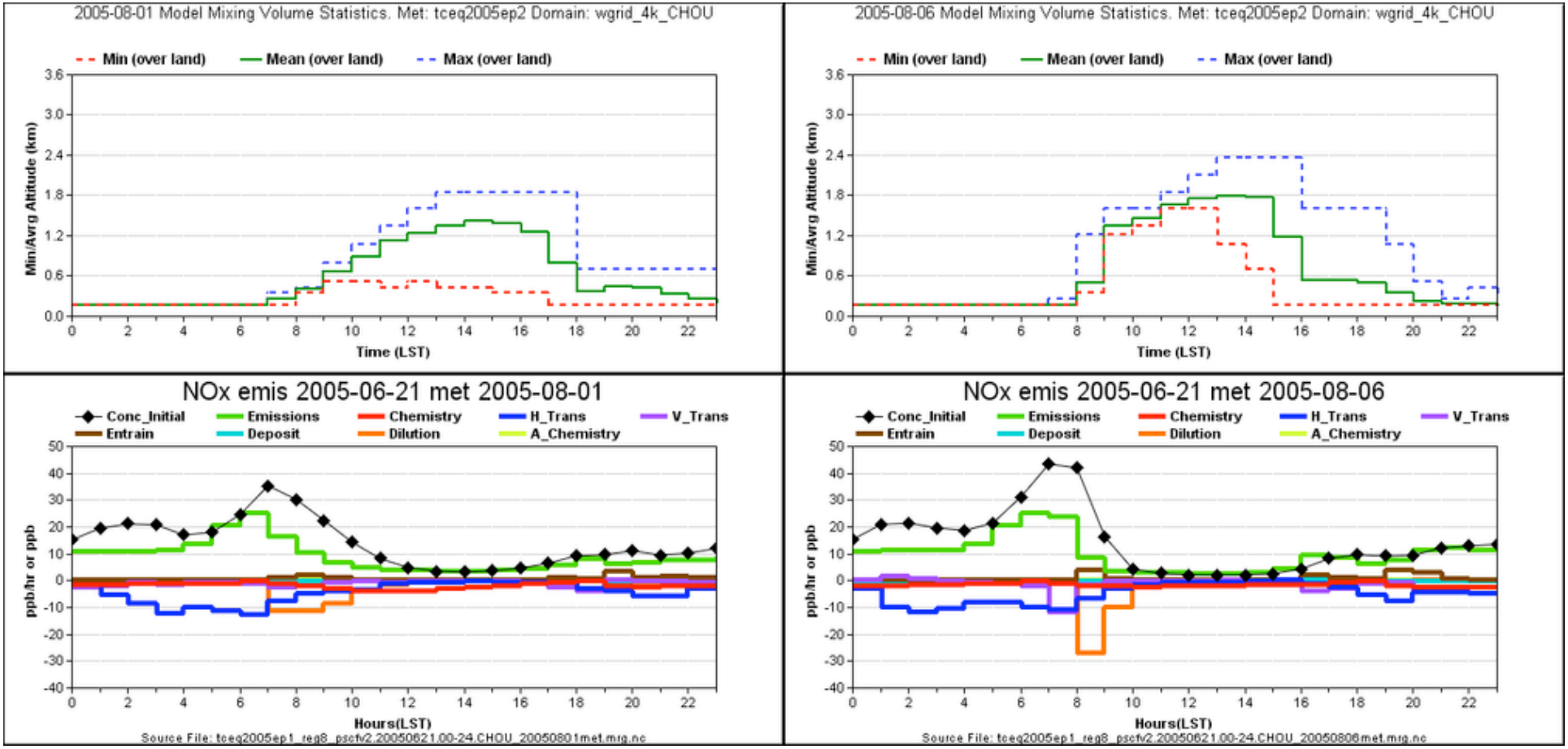


Slow Riser

Fast Riser

Physical Processes : NOx

06/21/05 Weekday

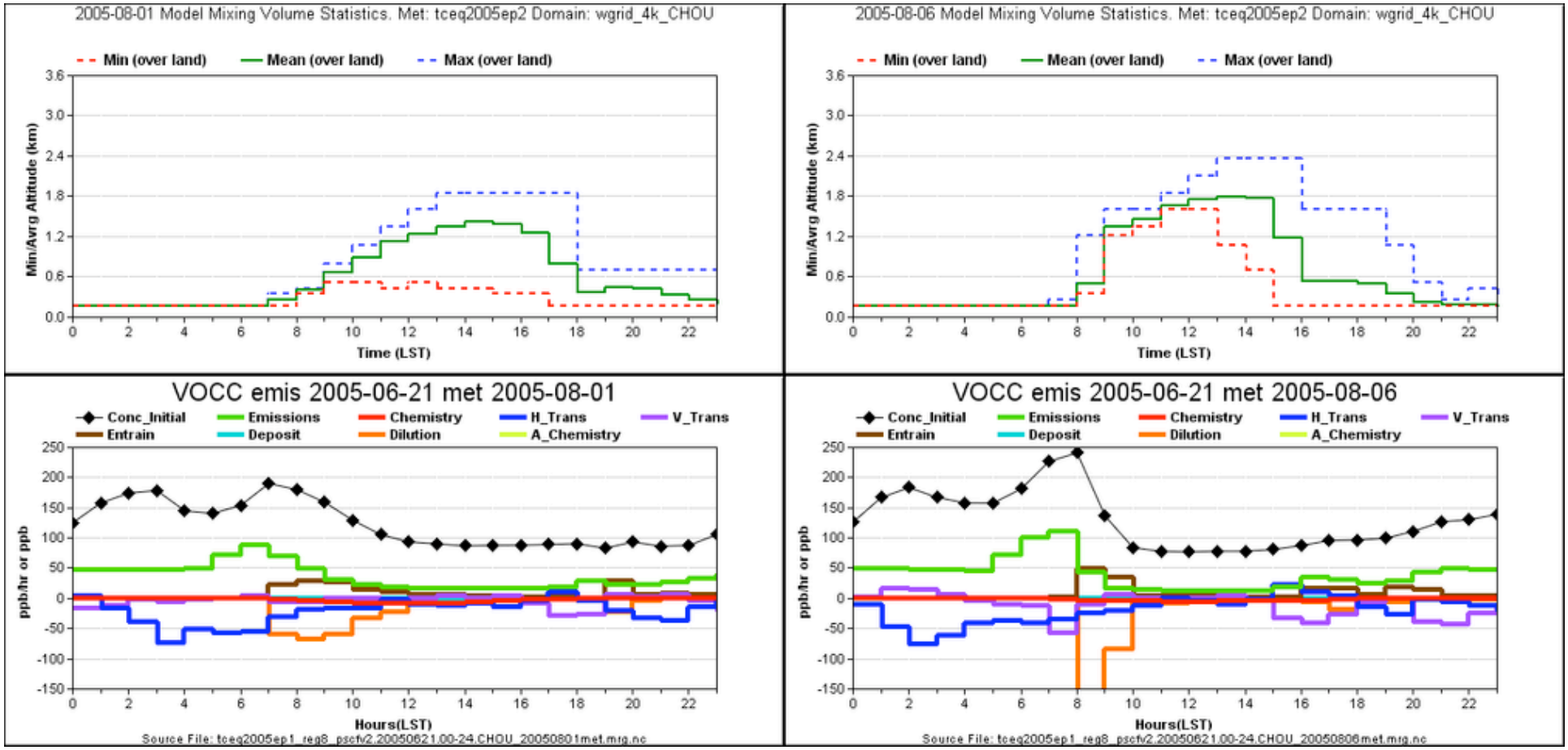


Slow Riser

Fast Riser

Physical Processes : VOC

06/21/05 Weekday



Slow Riser

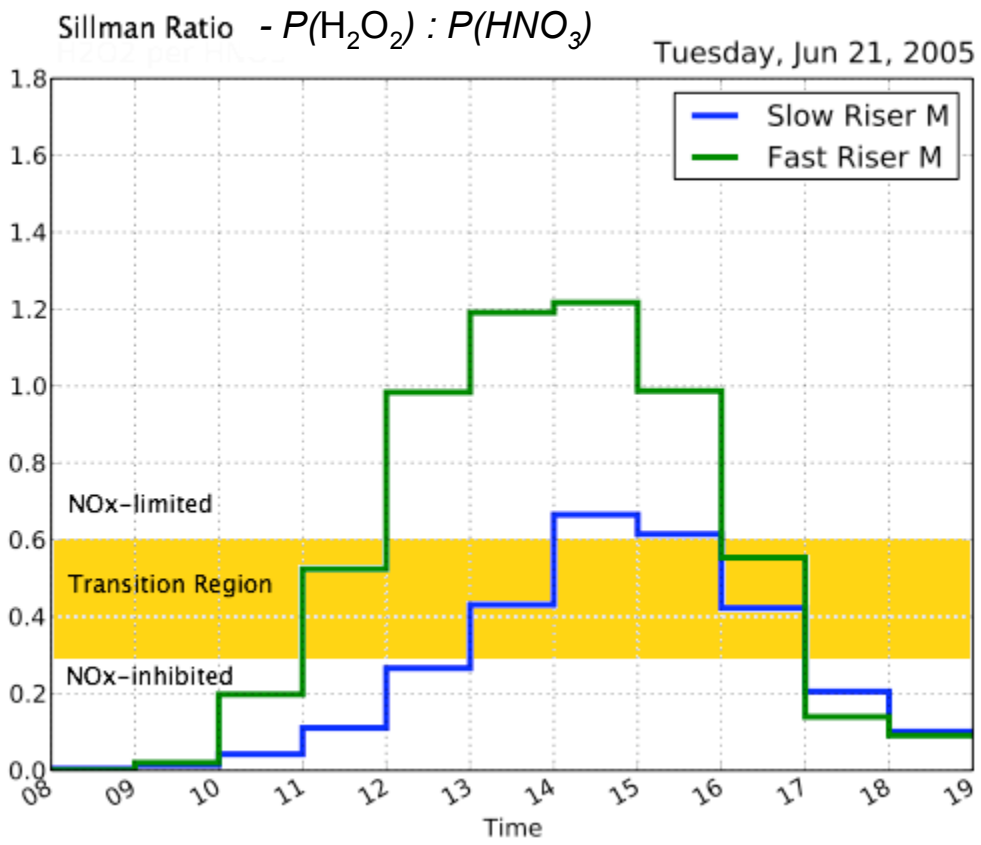
Fast Riser

Chemical Processes

- Aggregated for photochemical day
- Sources of new OH radicals virtually the same
- Shift of OH reactions from OH+NO2 to OH+VOC in PBL FAST
- Shift of OH+VOC to slower reacting species in PBL FAST
- Production of late afternoon H2O2 production in PBL FAST

Fast Riser NOx-limited Earlier, Longer

Weekday



NOx-limited

$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$

NOx-inhibited

$OH + NO_2 \rightarrow HNO_3$

Summary and Conclusion

- Fast Riser vs. Slow Riser
  - Entrainment of VOCs that bring in new VOCs
  - 5x more Dilution of NOx and VOCs
  - Steeper O3 production rate
  - NOx-limited much earlier in day than Slow Riser
  - Lower & Earlier Peak O3

- Same set of EI show distinct O3 producing regimes
  - Affect the type of controls needed to reduce O3

Future Work

- Compare Slow Riser and Fast Riser phenomena with Observed data.
- Evaluation of ACM2 mixing scheme in Houston

Acknowledgements

This project was funded by the Houston Advanced Research Center (HARC) under Project H97.

www.harc.edu

Thanks to TCEQ for providing data and guidance.

Questions