Seven air quality forecasts and their ensemble: Upper-air comparisons with O_3 and aerosol lidar data during the TexAQS-2006 field study

***S. McKeen*[1,2], *C. Senff*[2], *R. Alvarez*[2], *V. Bouchet*[3], *W. Gong*[4], *S. Gaudreault*[3], *J. McHenry*[5], *J. McQueen*[6], *P. Lee*[7], *Y. Tang*[6], *G. Carmichael*[8], *G. Grell*[1,2], *S. Peckham*[1,2], *R. Ahmadov*[1,2], *S.-W. Kim*[1,2]

(1) Cooperative Institute for Research in Environmental Sciences, University of Colorado, Boulder, Colorado, USA ; (2) Earth System Research Laboratory, NOAA, Boulder, Colorado, USA ; (3) Meteorological Service of Canada, Environment Canada, Dorval, Quebec, Canada
(4) Science and Technology Branch, Environment Canada, Downsview, Ontario, Canada ; (5) Baron Advanced Meteorological Systems, Research Triangle Park, North Carolina, USA ; (6) EMC, National Center for Environmental Prediction, NWS/NOAA, Camp Springs, MD, USA
(7) Air Resources Laboratory, National Oceanic and Atmospheric Administration, Camp Springs, MD, USA ; (8) Center for Global and Regional Environmental Research, University of Iowa, Iowa City, Iowa, USA

Introduction:

As part of the 2006 Texas Air Quality Study/Gulf of Mexico Atmospheric Composition and Climate Study (TexAQS-2006/GoMACCS), the TOPAZ lidar instrument was flown aboard one of NOAA's Twin Otter aircraft from the beginning of August to mid September. This platform provides high spatial and temporal resolution data for upper-air O_3 evaluations from over the larger East Texas region in general, and the Houston urban corridor in particular. This work summarizes comparisons of several air quality forecast models, and their ensemble, with observations from the 2006 TOPAZ O_3 lidar and PBL data-set.
This analysis compliments previous evaluations of the same air quality models based on in-situ sampling from the NOAA WP-3 aircraft and surface network data (McKeen et al., 2009; Wilczak et al., 2009; Djalalova et al., 2009). Day-by-day statistics and summary statistics for each model are available on a public web-site.

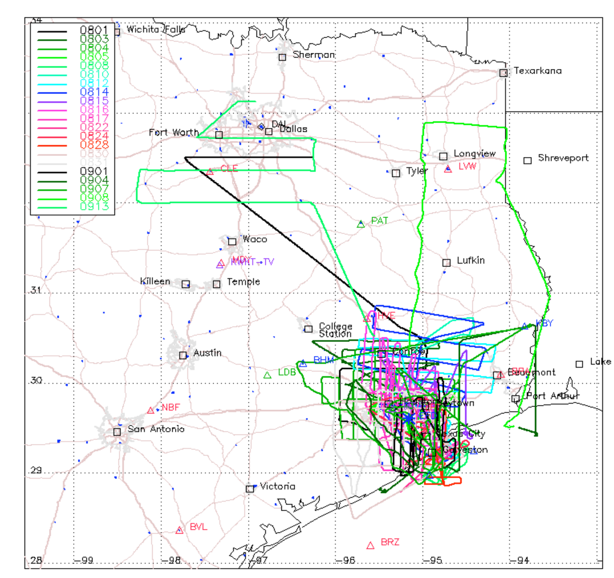
AQ forecast model evaluation web-site:
http://www.esrl.noaa.gov/csd/2006/modeleval/topaz/

TOPAZ: NOAA's airborne Ozone/Aerosol Lidar
Tunable Optical Profiler for Aerosols and oZone)

- Compact, light-weight, all solid state lidar
- 3 tunable UV wavelengths
- Designed for deployment on NOAA Twin Otter
- Measures O_3 and aerosol backscatter profiles
- Altitude coverage: from near the surface to ~2.5 km ASL

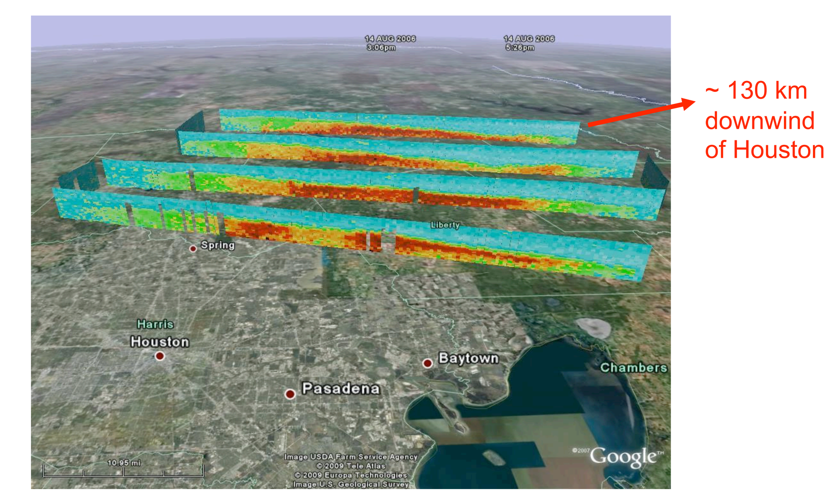
Ozone
- Precision: 3-15 ppb
- Resolution: 90 m vertical, 700 m horizontal

Aerosol backscatter (300 nm)
- Uncalibrated
- Resolution: 6 m vertical, 700 m horizontal
- **Used to determine PBL heights** (through wavelet analysis)



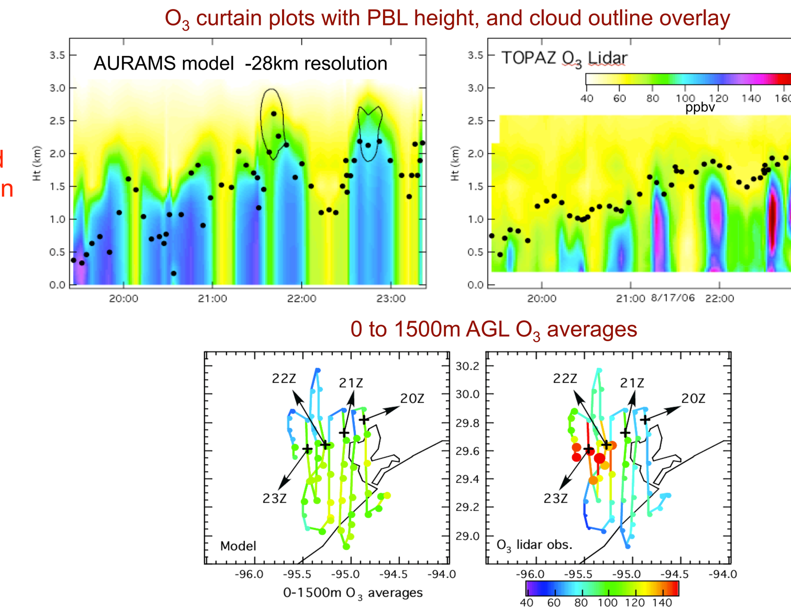
TOPAZ data web-site:
http://www.esrl.noaa.gov/csd/lidar/texaqs06/topaz/

Example: TOPAZ ozone data from 14 Aug 2006



Example of daily comparison plots on evaluation web-site 8/17/06

O_3 curtain plots with PBL height, and cloud outline overlay



Real-time AQ Model Forecasts Collected during TexAQS-II:

- 12km and 36km WRF/Chem (NOAA/GSD) - NEI-99
  PBL heights from model diagnosis, Cloud water
  Recent retrospective runs – 27km, 20km (PBL only) and 4km (PBL only)
- 12km CMAQ/WRF-NMM (NCEP) - NEI-2001, (Pouliot – EPA)
  PBL heights from model diagnosis, Cloud water
- 21km Canadian CHRONOS model (GEMS) - NEI-2001
  No PBL heights, No meteorological fields
- 28km Canadian AURAMS model (GEMS) - NEI-2001
  PBL heights from model diagnosis, Cloud water
- 5km and 15km Baron AMS MAQSIP model (MM5) - NEI-2001, (Vukovich – BAMS)
  PBL heights determined from meteorological output, Cloud Water
- 12km U. of Iowa STEM model (WRF)- NEI-2001, (Vukovich – BAMS)
  PBL heights determined from meteorological output, No Cloud Water
  Boundary conditions from RAQMS global model and 60km U.S. domain
- Ensemble of eight models, O_3, PBL heights, and meteorology
  5, 10, 15, 20, 25 and 30 km horizontal resolution

Some details of the statistical analysis

- Only days with 3 or more hours of available lidar data – 12 out 21 flights

For O_3

- O_3 lidar bins averaged over model grid cells – nearest neighbor, no interpolation
- Vertically, require >50 % overlap between model levels and range gates
- For summary comparisons, must have > 300 samples at any level.

For PBL heights

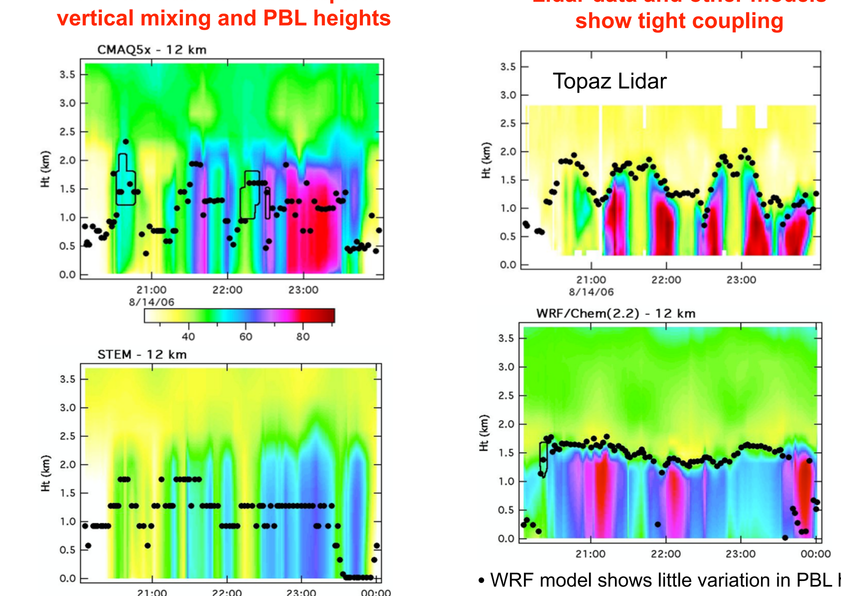
- Only compare when local time before 5:30 pm (22:30 UTC)

For Model Ensemble

- Pre-defined lat-lon girds (~5km to 30km horizontal) with high vertical resolution
- Model results averaged over ensemble grids – nearest neighbor, no interpolation
- Vertically, require >50 % overlap between model levels and range gates

Correspondence between PBL mixing and PBL depth

Two models have uncoupled vertical mixing and PBL heights / **Lidar data and other models show tight coupling**

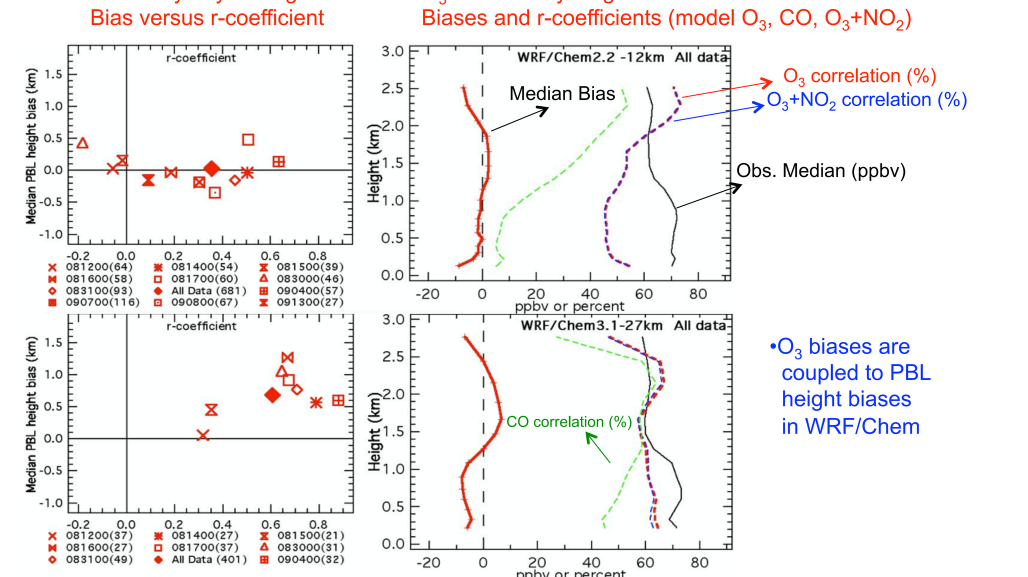


- WRF model shows little variation in PBL height

Qualitative and quantitative consistency with McKeen et al. (2009); Wilczak et al. (2009)

TOPAZ O_3 Lidar and PBL height summary Statistics
WRF/Chem version 2.2 versus WRF/Chem 3.1

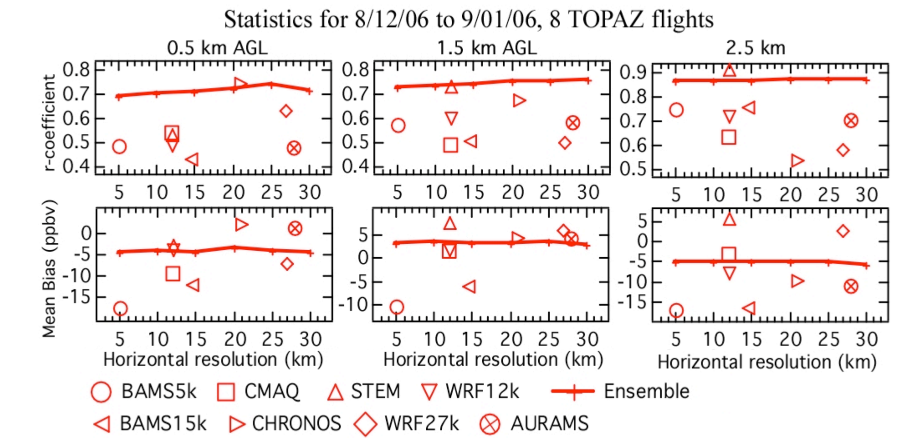
Boundary Layer Height Bias versus r-coefficient / O_3 statistics by height: Biases and r-coefficients (model O_3, CO, O_3+NO_2)



- O_3 biases are coupled to PBL height biases in WRF/Chem

O_3 Statistical Comparisons with Lidar Data – 3 different heights
r-coefficients and Mean Bias

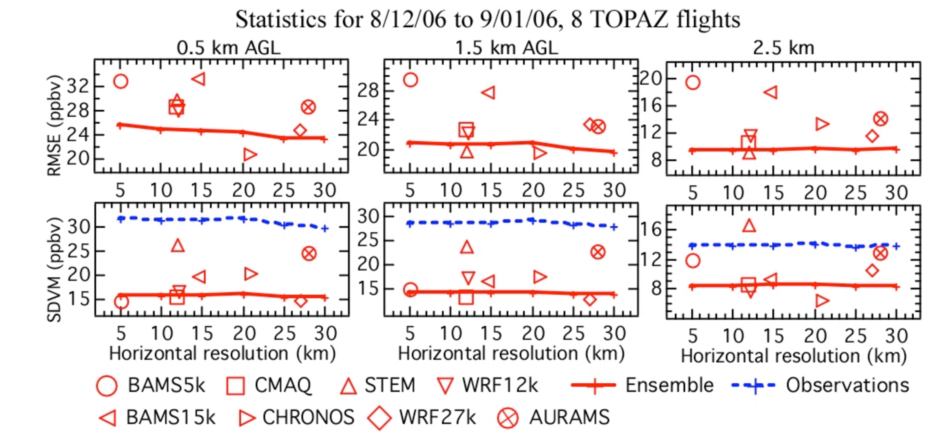
Statistics for 8/12/06 to 9/01/06, 8 TOPAZ flights



- 0.5 km results similar to surface analysis (McKeen et al., 2009) only CHRONOS shows reasonable correlation and bias
- At 1.5 and 2.5 km the STEM model shows high correlation, and 5 ppbv bias
- The model Ensemble gives (almost) the best correlations – no resolution dependence

O_3 Statistical Comparisons with Lidar Data – 3 different heights
RMSE and Variance about the Mean

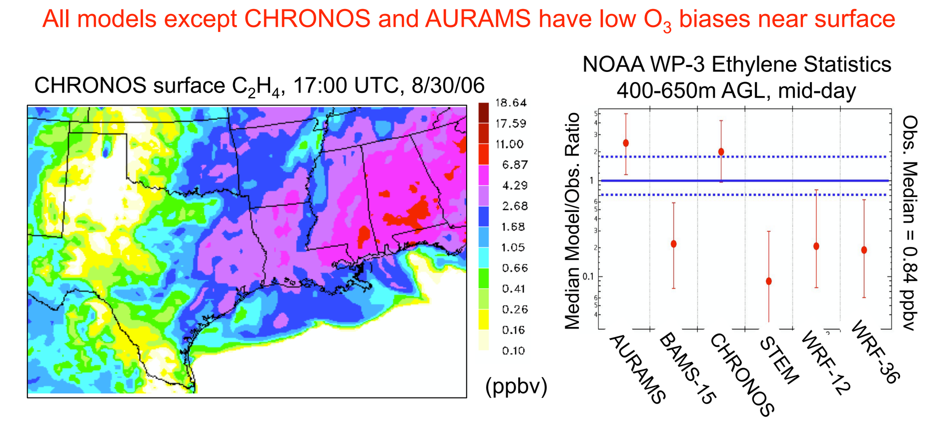
Statistics for 8/12/06 to 9/01/06, 8 TOPAZ flights



- RMSE are largely dominated by model biases
- The model Ensemble gives (almost) the lowest RMSE, but is too "smooth"

Reasons for good model performance:

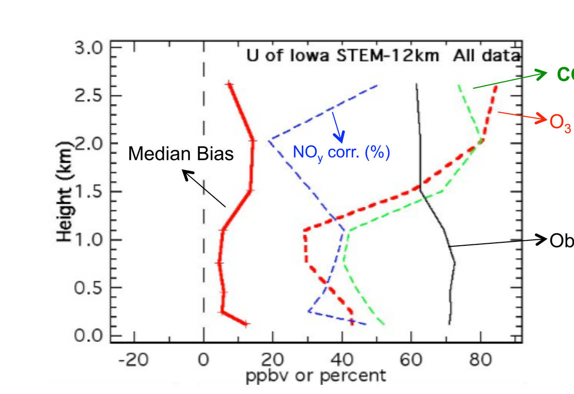
All models except CHRONOS and AURAMS have low O_3 biases near surface



Ethylene has biogenic source from simplified Isoprene Chemistry: Isoprene + OH → $2C_2H_4$

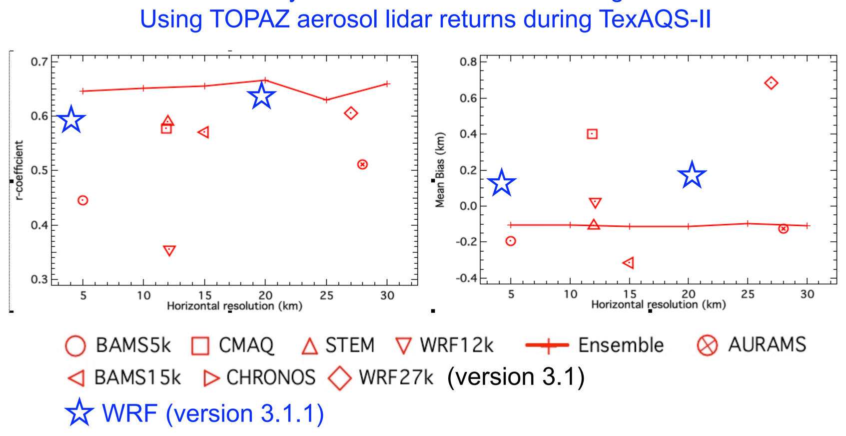
Highly reactive VOC environment yields higher O_3 formation rates

At higher altitude – the STEM model considers distant transport through coupling with the RAQMS global transport model (Pierce et al., 2007)



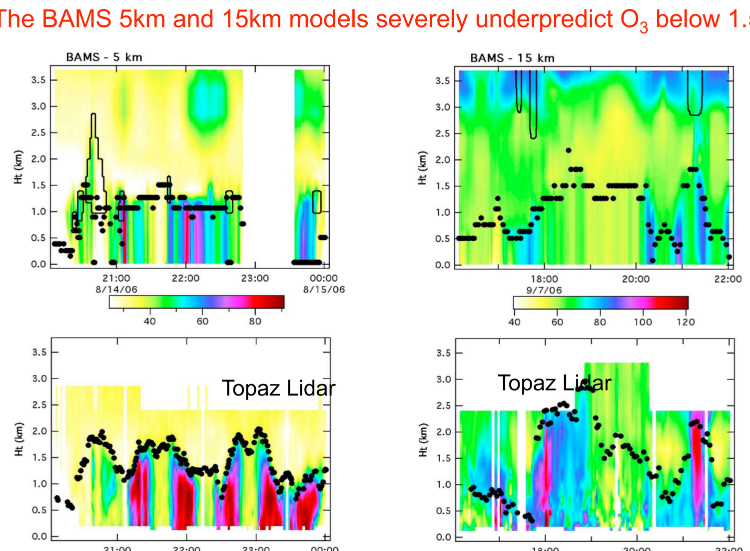
High positive correlation with CO above 1.5 km implies variance due to distant anthropogenic forcing is captured by RAQMS/STEM

Summary Model Statistics for PBL heights
Using TOPAZ aerosol lidar returns during TexAQS-II



- Latest versions of WRF show much improved PBL heights

The BAMS 5km and 15km models severely underpredict O_3 below 1.5 km



- Lidar comparisons suggest too much cloudiness and venting of boundary layer pollutants
- Low Temperature biases (WP-3 comparisons), low PBL heights

Conclusions:

The TOPAZ data during TexAQS-II are used to infer:

1) PBL height biases and O_3 biases are coupled (in most models)
2) The 3-dimensional model Ensemble yields consistently good results
3) Reasons for reduced model performance:
   BAMS – too cloudy, too much convection
   CMAQ – uncoupled PBL transport with meteorology
   WRF/Chem – poor PBL dynamics (land-use issues) with WRF version 2.2
4) Reasons for good model performance
   CHRONOS (< 1.5 km) – High reactive VOC emissions in Houston area
   STEM (> 1.5 km) – Coupling of global model into regional AQ forecasts

References:

McKeen, S., et al. (2009). "An evaluation of real-time air quality forecasts and their urban emissions over eastern Texas during the summer of 2006 TexAQS field study." , JGR, 114, D00F11

Wilczak, J., et al. (2009), "Evaluation of Meteorology and Surface Ozone in NMM-CMAQ and WRF-Chem Simulations During the TexAQS II Field Program", JGR, 114, D00F14.

Pierce, R. B., et al. (2007), "Chemical data assimilation estimates of continental U.S. O_3 and nitrogen budgets during ICTE-North America", JGR, 112, D12S21.

Djalalova, I., et al. (2009), "Ensemble and bias-correction techniques for AQ model forecasts of surface O_3 and PM2.5 during the TEXAQS-II experiment of 2006", accepted in Atmos. Envir