Model Performance Evaluation Using R. V. Ronald H. Brown Data

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Southeast Texas Photochemical Modeling Technical Committee
January 26, 2010
Background

• The NOAA RV Ron Brown arrived in the HGB area on August 15, 2006, and collected data until its departure on September 13.

• The ship carried a wide array of sampling platforms onboard and provided extensive data collected in the Gulf of Mexico, Galveston Bay, and in the Houston Ship Channel.

• The Ron Brown data provides a unique opportunity to evaluate CAMx model performance in areas not usually monitored.
R.V. Ron Brown Instrumentation

PMEL VAN3 -
Aerosol composition:
Organic speciation (PTR-MS)
NR composition (WTOF-AMS)
Radiometers

PMEL VAN1 -
Aerosol composition:
Ions (PILS-IC)
Water sol. organics (PILS-TOC)
Organic speciation (PILS-LCMS)
NR speciation (AMS)
OC/EC
CCN
SO2, O3

PMEL VAN2 -
Aerosol parameters:
Number and size distribution
Light scattering (Neph)
Scattering f(RH) (Neph)
Light absorption (PSAP)
Light extinction (CarDS)
Extinction f(RH) (CarDS)
Light absorption (PAS)
Composition (impactors)
Functional groups (FTIR)
Radon

ESRL VAN3 -
NO; NO2; NOy; PANs; HNO3; O3; CO;
CO2; SO2; jNO2; jO3; jNO3; met; GPS/AIS

ESRL VAN2 -
VOCs: GC-MS; PTR-MS; CH2O
Alkyl N; NO3; N2O5; HO2/RO2

ESRL VAN1 -
Gas-phase inlets and
radiometers tower

2006 TexAQS GoMACCS
## R.V. Ron Brown Instrumentation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Photolysis rates (j-values)</td>
<td>Spectral radiometer</td>
</tr>
<tr>
<td>Ozone (O3)</td>
<td>UV absorbance</td>
</tr>
<tr>
<td>Ozone</td>
<td>NO chemiluminescence</td>
</tr>
<tr>
<td>Carbon monoxide (CO)</td>
<td>Nondispersive IR</td>
</tr>
<tr>
<td>Carbon dioxide (CO2)</td>
<td>Nondispersive IR</td>
</tr>
<tr>
<td>Sulfur dioxide (SO2)</td>
<td>Pulsed UV fluorescence</td>
</tr>
<tr>
<td>Nitric oxide (NO)</td>
<td>Chemiluminescence</td>
</tr>
<tr>
<td>Nitrogen dioxide (NO2)</td>
<td>Photolysis/chemiluminescence</td>
</tr>
<tr>
<td>Total reactive nitrogen oxides (NOy)</td>
<td>Au tube/chemiluminescence</td>
</tr>
<tr>
<td>Peroxyacyl nitric anhydrides (PANs)</td>
<td>Gas Chromatograph (GC)/Electron Capture Detector (ECD)</td>
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<tr>
<td>Alkyl nitrates (RONO2)</td>
<td>GC/Mass Spectrometer (GC/MS)</td>
</tr>
<tr>
<td>Nitrate radical (NO3); Dinitrogen pentoxide (N2O5)</td>
<td>Cavity ring-down spectrometry</td>
</tr>
<tr>
<td>Nitric acid (HNO3)</td>
<td>Mist chamber/Ion Chromatograph</td>
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<tr>
<td>Water vapor (H2O)</td>
<td>Nondispersive IR</td>
</tr>
<tr>
<td>Continuous Speciation of VOCs</td>
<td>PTR-MS/Chem Ionization MS</td>
</tr>
</tbody>
</table>
### Ron Brown Instrumentation (Cont.)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>VOC Speciation</td>
<td>GC/MS</td>
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<tr>
<td>Formaldehyde (HCHO)</td>
<td>1,3-cyclohexanedione (CHD) fluorimetry</td>
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<td>Radon (Rn)</td>
<td>Radon gas decay</td>
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<td>Seawater/atmospheric CO2</td>
<td>Nondispersive IR</td>
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<tr>
<td>Enhanced measurement of radiative fluxes</td>
<td>Spectral radiometers</td>
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<tr>
<td>Aerosol optical depth</td>
<td>Total Ozone Portable Spectrometer (MicroTOPS)</td>
</tr>
<tr>
<td>Irradiance</td>
<td>Portable Radiation Package (PRP)</td>
</tr>
<tr>
<td>Size-resolved aerosol composition and gravimetric mass</td>
<td>Impactors (Ion Chromatograph (IC), X-Ray Fluoresence (XRF), and thermal-optical OC/EC)</td>
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<tr>
<td>Organic Carbon/Elemental Carbon (OC/EC)</td>
<td>On-line thermal optical</td>
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<tr>
<td>Ionic Aerosol Composition</td>
<td>Particle Into Liquid Sampler (PILS)</td>
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<tr>
<td>Aerosol Size and Composition</td>
<td>Aerosol Mass Spectrometer</td>
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<tr>
<td>Organic function groups</td>
<td>Fourier Transform Infrared spectrometer (FTIR)</td>
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<tr>
<td>Aerosol scattering (400, 550, 700 nm)</td>
<td>TSI Model 3563 Nephelometer</td>
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</tbody>
</table>
## Ron Brown Instrumentation (Cont.)

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<tr>
<th>Parameter</th>
<th>Method</th>
</tr>
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<tr>
<td>Aerosol absorption (400, 550, 700nm)</td>
<td>Radiance Research Particle Soot Absorption Photometer (PSAP)</td>
</tr>
<tr>
<td>Aerosol number</td>
<td>Condensation Nuclei Counter (CNC)</td>
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<tr>
<td>Aerosol size distribution</td>
<td>Twin Differential Mobility Analyzers (DMA) and an Aerodynamic Particle Sizer (APS)</td>
</tr>
<tr>
<td>Aerosol light scattering hygroscopic growth f(RH)</td>
<td>Twin TSI 3563 nephelometers</td>
</tr>
<tr>
<td>Aerosol size hygroscopic growth g(RH)</td>
<td>Tandem DMAs</td>
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<tr>
<td>Aerosol light extinction hygroscopic growth f(RH)</td>
<td>Cavity ring-down spectrometer</td>
</tr>
<tr>
<td>Total and sub-micron aerosol extinction</td>
<td>Cavity ring-down spectrometer</td>
</tr>
<tr>
<td>Ozone/aerosol vertical profiles</td>
<td>O3/Aerosol Lidar (OPAL)</td>
</tr>
<tr>
<td>Wind/temperature vertical profiles</td>
<td>915 MHz wind Radar</td>
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<tr>
<td>High-resolution Boundary Layer (BL) winds/aerosol</td>
<td>High-Resolution Doppler Lidar (HRDL)</td>
</tr>
<tr>
<td>Wind profiles/microscale turbulence</td>
<td>C-band radar</td>
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<tr>
<td>Temperature/relative humidity profiles</td>
<td>Radiosondes</td>
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<tr>
<td>Surface energy balance (fluxes)</td>
<td>Eddy covariance (bow mounted)</td>
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<tr>
<td>High resolution BL turbulence structure</td>
<td>Doppler mini-Sodar</td>
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</table>
## CAMx Ozone Modeling in SIP Development

### The Big Picture

<table>
<thead>
<tr>
<th>Case</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td><strong>Base Case</strong></td>
<td>Day-specific emissions; replicate what actually happened</td>
</tr>
<tr>
<td><strong>Baseline Case</strong></td>
<td>Typical emissions; used in RRF to predict future design values</td>
</tr>
<tr>
<td><strong>Future Base Case</strong></td>
<td>Apply future growth + on-the-books controls to estimate future ozone</td>
</tr>
<tr>
<td><strong>Control Strategy Testing</strong></td>
<td>Determine control strategies that will effectively reduce ozone</td>
</tr>
<tr>
<td><strong>SIP</strong></td>
<td>Document modeling procedures</td>
</tr>
</tbody>
</table>
The Voyage of the Ron Brown

- Performance analysis using the Ron Brown data was complicated by the course taken by the ship, since it frequently traversed almost identical paths, sometimes several times within a single day.

- Model performance was simplified somewhat by segregating the data into seven distinct analysis zones, allowing model performance to be evaluated in each of seven different environments.
NOAA RV Ron Brown Measured O3 Mixing Ratios
15AUG 00:00 to 11SEP 12:30, 30 Minute Averages

Maximum Observed O3:
168.03 ppbV

NOx Point Source Locations
Analysis Zones

- **Houston Ship Channel.** This zone was defined as consisting of all measurements made to the north and west of Barbour’s Cut, and is the portion of the Houston Ship Channel which bisects the main industrial area of eastern Harris County. The Ron Brown made an extended visit to this area on September 6 and 7, including an overnight stay at Jacinto Port.

- **Barbour’s Cut.** The Ron Brown made seven extended visits to Barbour’s Cut near the northwestern extremity of Galveston Bay.

- **Barbour’s Cut to Galveston.** The ship made numerous transects of the deepwater channel between Barbour’s Cut and the mouth of Galveston Bay located between Galveston Island and Bolivar Peninsula. This channel is actually part of the Houston Ship Channel but is analyzed separately because it is not located directly in the industrial area.
Analysis Zones (cont.)

• **Galveston Harbor.** The Ron Brown collected data during two overnight stays in Galveston Harbor and also briefly during two other occasions. The ship also remained docked in the Galveston Harbor for three days between August 18 and 21 during which time no data were collected.

• **Galveston Entrance/Anchororage.** This zone consists of the main fairway through which ships approach the entrance to Galveston Bay and parts of two anchorage areas lying alongside the fairway. This zone was treated separately from other offshore locations because the Ron Brown conducted extensive sampling of ship emissions in this area.
Analysis Zones (cont.)

• **Gulf – Near Shore.** The Near Shore area of the Gulf of Mexico consists of measurements made within approximately 20 kilometers of the Texas Coast (excluding the Galveston Entrance Anchorage area). This zone is intended to represent the offshore areas affected directly by onshore emissions carried out to sea by the land breeze.

• **Gulf – Offshore.** This zone is defined by measurements made by the Ron Brown in the Gulf of Mexico farther than approximately 20 kilometers from shore. This area is intended to be representative of marine background.

• The ship made brief visits to ports at Freeport and Palacios, but these small data sets were not included in this analysis.
Houston Ship Channel

**Observed and Modeled O3 Mixing Ratios**
Houston Ship Channel, 5 Minute Averages

*Note: Consistent with NOAA’s preferred notation, graphics depicting data from the R.V. Ron Brown use the term “Mixing Ratio” instead of “Concentration.” In this context the two terms are interchangeable.*
Segment C: Jacinto Port

Observed and Modeled O3 Mixing Ratios
06SEP 15:00 to 07SEP 11:10, 30 Minute Averages

Wind: (5 m/sec.)

O3 ppbV

Time

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Segment D: Turning Basin to Jacinto Port

NOAA RV Ron Brown Measured O3 Mixing Ratios
07SEP 11:20 to 07SEP 13:10, 5 Minute Averages

Segment E: Turning Basin to Barbour’s Cut

NOAA RV Ron Brown Measured O3 Mixing Ratios
07SEP 13:20 to 07SEP 16:35, 5 Minute Averages

CAMx Reg10 Modeled O3 Mixing Ratios
07SEP 11:20 to 07SEP 13:10, 5 Minute Averages

CAMx Reg10 Modeled O3 Mixing Ratios
07SEP 13:20 to 07SEP 16:35, 5 Minute Averages
Barbour’s Cut

Observed and Modeled O3 Mixing Ratios
Barbours Cut, 30 Minute Averages

Shaded Areas Represent Periods Modeled Without the 2- and 4-km Fine Grids.
Barbour’s Cut to Galveston
12-Hour Forward Trajectories
Beginning 00:00, August 8, 2006

Daily Max: 8hr O3 ppb at monitors
- 100 +
- 95 to < 100
- 90 to < 95
- 85 to < 90
- 80 to < 85
- 75 to < 80
- < 75

MetStat: Observed
MetStat: ep1b.ets.dbemis.fldcats.newuhsst.newutcs.mlulc.grel

Forward Trajectories 2006—09—08
Max 8hr O3 (monitored): 81.1 at KATP 8Hr frame: 1000—1700

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Galveston Harbor

Observed and Modeled O3 Mixing Ratios
Galveston Harbor, 30 Minute Averages

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Galveston Entrance/Anchorage

Observed and Modeled O3 Mixing Ratios
Galveston Entrance Anchorage, 5 Minute Averages

Time

O3 ppbV

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Gulf-Near Shore

Observed and Modeled O3 Mixing Ratios
Gulf - Near Shore, 30 Minute Averages
Gulf-Offshore

**Observed and Modeled O3 Mixing Ratios**
Gulf - Offshore, 30 Minute Averages

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PBL Analysis

- TCEQ recently received planetary boundary layer (PBL) depth estimates from Dr. Sara Tucker at NOAA, derived using the High-Resolution Doppler LiDAR (HRDL) instrument located on the stern of the Brown.

- These data were compared with modeled PBL depths to see how well the model captures this important meteorological parameter.

- Two analysis zones were used:
  - Gulf = Galveston Entrance/Anchorage ∪ Near Shore ∪ Offshore
  - Galveston Bay = Houston Ship Channel ∪ Barbour’s Cut ∪ Barbour’s Cut to Galveston ∪ Galveston Harbor
Observed and Modeled PBL
15AUG 00:00 to 11SEP 12:30, 30 Minute Averages
Summary

• Ozone
  – The model tended to over-predict observed ozone concentrations below 50 to 60 ppb in all areas.
  – In the Galveston Bay area, the model under-predicted higher ozone concentrations, including some very high observed concentrations ranging up to 180 ppb+.
  – Outside Galveston Bay, the model was relatively unbiased for higher observed concentrations, and slightly over-predicted ozone concentrations in the Offshore zone.

• NO
  – The model under-predicted observed NO concentrations within the Galveston Bay area, especially large NO “spikes” apparently associated with local sources.
  – Outside the Bay, NO predictions were relatively unbiased.
Summary (cont.)

• **NO$_2$**
  - The model overall performed quite well for NO$_2$ in all areas.

• **HNO$_3$**
  - A large amount of scatter in the data pairs means that the model did not predict individual points very well, but the model showed little evidence of overall bias in its nitric acid predictions.

• **PAN**
  - In the Houston Ship Channel, measured PAN concentrations were close to the modeled values.
  - In most other situations, modeled PAN values showed a small positive bias, excepting a couple of dozen very high measured values in the Barbour’s Cut to Galveston zone.
  - In the Offshore region, modeled PAN concentrations were on the order of 2-3 times the observations.
Summary (cont.)

• **CO**
  – The model showed a positive bias of ~ 40% in most areas.
  – Model bias was ~10% during a brief visit to the Ship Channel.

• **ETH**
  – The model under-predicted ethylene concentrations by around a factor of two in the Ship Channel and in the Barbour’s Cut to Galveston zones.
  – The model was unbiased in Barbour’s cut except for concentrations < 1 ppb.
  – Modeled and observed concentrations of ethylene outside Galveston Bay were fairly low, with only a few observations > 2 ppb.
Summary (cont.)

• **ISOP**
  – Unusually high isoprene concentrations measured in the Ship Channel were not replicated by the model.
  – Otherwise, the model showed little bias in the Ship Channel and in Barbour’s Cut.
  – Elsewhere, both observed and modeled concentrations were generally very low (< 1 ppb).

• **FORM**
  – Overall model performance was good, except for some very high observations in the Galveston Bay area which were not captured by the model.
Summary (cont.)

• PBL
  – Modeled PBL shows little evidence of bias.
  – In Galveston Bay area, both modeled and observed PBLs have a wider dynamic range than in the Gulf.
  – Large (> 800 m) values of modeled and observed PBL in the Gulf are often associated with land breeze advection.