HGB SIP Modeling Update
Initial TexAQS II Episodes Modeling

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Air Modeling Team
Air Modeling & Data Analysis Section

October 7, 2008
(corrected 11/21/08)
CAMx Ozone Modeling in SIP Development
The Big Picture

- **Base Case**: Day-specific meteorology and emissions; replicate what actually happened
- **Baseline Case**: Day-specific meteorology and Typical emissions; used in RRF to predict future design values
- **Future Base Case**: Apply future growth + on-the-books controls to estimate future ozone
- **Control Strategy Testing**: Determine control strategies that will effectively reduce ozone
- **SIP**: Document modeling procedures

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CAMx Ozone Modeling in SIP Development
Base Case – Historical Episode Replication

Meteorological Modeling
Winds, Mixing Depth, Temperature, etc.

Emissions Modeling
VOC, CO & NO$_x$
Point, Area, on- & Non-Road & Biogenic

CAMx Modeling
O$_3$, NO$_x$, VOC, CO, etc.
Chemical Mechanism (CBIV, CB05), “Mixing” schemes

Evaluate CAMx Performance
(How well does the model replicate the episode?)
Bias, Time Series, Contour Plots

Suitable Base Case
## TexAQS II Monitored Ozone
### July and August 2006

<table>
<thead>
<tr>
<th>Date</th>
<th>hgb daily max 8-h ozone (ppb)</th>
<th># of sites &gt;= 85ppb</th>
</tr>
</thead>
<tbody>
<tr>
<td>20060701</td>
<td>51.8</td>
<td>1</td>
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<tr>
<td>20060704</td>
<td>42.3</td>
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<tr>
<td>20060719</td>
<td>80.1</td>
<td>1</td>
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<td>20060722</td>
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<td>20060725</td>
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<td>20060731</td>
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<tr>
<td>20060630</td>
<td>88.8</td>
<td>1</td>
</tr>
</tbody>
</table>

The graph shows the daily maximum 8-hour ozone levels and the number of sites exceeding 85 ppb for each day from July 1 to August 31, 2006.
TexAQS II Episode Selection

• Met modeling for the TexAQS II episodes
  – August 13 through August 23, 2006
  – August 27 through September 15, 2006
  – September 16 through September 30, 2006
  – October 1 through October 12, 2006

• EI modeling for the TexAQS II episodes
  – August 15 through September 15, 2006
  – September 16 through October 11, 2006

• CAMx modeling for the TexAQS II episodes
  – August 15 through August 22, 2006
  – August 29 through September 8, 2006
  – September 12 through September 14, 2006
  – September 19 through September 20, 2006
  – September 25 through September 27, 2006
  – October 3 through October 11, 2006
Met Modeling for TexAQS II Episodes

Met modeling for the TexAQS II episodes includes:

- New UT-CSR land use/land cover (LU/LC) data
- Latest QA’d radar profiler observation-nudging data
- Hourly sea surface temperatures, U of H
Met Modeling for the TexAQS II Episodes
August 13 through August 23, 2006

Wind Speed and Wind Direction
Scatter Plots

Houston–Galveston – Region 12 Average

Houston–Galveston – Region 12 Average
Met Modeling for the TexAQS II Episodes
August 13 through August 23, 2006
Met Modeling for the TexAQS II Episodes
August 13 through August 23, 2006
EI Modeling for the TexAQS II Episodes

- **Hourly Emissions**
  - 2006 Special EI: August 15 through September 15, 2006
  - EPA Acid Rain Database (ARD): every day
  - TCEQ tank landing loss survey: event days
  - GloBEIS biogenics with satellite PAR and temperature: every day

- **Daily Emissions**
  - Texas Forest Service fires: event days
  - On-road mobile emissions, as per TTI: day-type

- **Ozone Season Day (OSD) Emissions**
  - 2006 STARS point sources
  - NMIM 2006 non-road mobile sources
  - 2005 TexAER with appropriate growth off-road and area sources
  - PSCFv2 emissions reconciliation
EI Modeling for the TexAQS II Episodes
Weekday (8/17/06) and Sunday (8/20/06) NOX

Diurnal Profile
EI Modeling for the TexAQS II Episodes

Weekday and Sunday NO\textsubscript{x} Emissions by Source Category

Weekday (Aug 17 & Sept 27) and Sunday (Aug 20 & Oct 8)

Selected Weekdays and Sundays Dates

- Biogenic
- Marine
- Area
- Non-Rd
- On-Rd
- Low-Pt
- TLL
- TFS-Fire
- El-Pt

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EI Modeling for TexAQS II Episodes
Weekday (8/17/06) and Sunday (8/20/06) VOC
EI Modeling for TexAQS II Episodes
Weekday and Sunday VOC

Weekday (Aug 17 & Sept 27) and Sunday (Aug 20 & Oct 8)
VOC Emissions by Source Category

VOC Emissions in TPD

Selected Weekdays and Sundays

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CAMx Modeling for the TexAQS II Episodes

• **Statistical Performance Evaluations**
  – Peak 1-hour and 8-hour ozone concentrations
  – Relative bias (%) 1-hour ozone > 60 ppb and site average peak 8-hour ozone
  – Relative error (%) 1-hour ozone > 60 ppb and site average peak 8-hour ozone

• **Graphical Performance Evaluations**
  – Time series of measured vs modeled 1-hour ozone for selected sites
  – Time series of measured vs modeled precursors for selected sites
  – Time Series of measured vs modeled 8-hour daily max for selected sites
  – Daily maximum 8-hour ozone tile plots for selected episode days
  – Scatter-plots of ETH, OLE and IOLE for selected sites
Statistical Performance Evaluations

Modeled vs monitored peak ozone concentrations

Modeled vs monitored relative bias

Modeled vs monitored relative error
### Monitored vs Modeled Peak Hourly Ozone Concentration

**TexAQS II Episodes**

<table>
<thead>
<tr>
<th>Episode Date</th>
<th>Monitored PK</th>
<th>Modeled PK</th>
<th>Monitored +20% PK</th>
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<tbody>
<tr>
<td>8/1</td>
<td>141.9</td>
<td>158.9</td>
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<tr>
<td>5/200</td>
<td>107.5</td>
<td>102.5</td>
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<td>10/200</td>
<td>82.3</td>
<td>107.8</td>
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<tr>
<td>11/200</td>
<td>83.3</td>
<td>109.7</td>
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</table>

**Episode Date**

- 8/1
- 5/200
- 6/200
- 7/200
- 8/200
- 9/200
- 10/200
- 11/200

### Monitored vs Modeled 8-Hour Ozone Concentrations

**TexAQS II Episodes**

<table>
<thead>
<tr>
<th>Episode Date</th>
<th>Monitored PK</th>
<th>Modeled PK</th>
<th>Ozone NAAQS</th>
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<tbody>
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<td>8/15/200</td>
<td>110.5</td>
<td>110.5</td>
<td>75</td>
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**Episode Date**

- 8/15/200
- 8/16/200
- 8/17/200
- 8/18/200
- 8/19/200
- 8/20/200
- 8/21/200
- 8/22/200
- 8/23/200
- 8/24/200
- 8/25/200
- 8/26/200
- 8/27/200
- 8/28/200
Graphical Performance Evaluations

Modeled vs monitored time series

Modeled vs monitored daily maximum 8-hour ozone

Modeled vs monitored HRVOC scatter plots
Air Quality Monitoring Sites in the HGB Area
Time Series of Daily Maximum 8-hour Ozone
Daily Maximum 8-Hour Ozone Modeled vs Monitored

Aug 17, 2006

Sept 1, 2006

Sept 7, 2006

Sept 14, 2006
Houston Ship Channel Auto-GC Monitors and HRVOC Point Sources (2006 Annual EI)
DRPK & WALV Measured vs Modeled CB05-HRVOC (ETH, OLE & IOLE)

Deer Park

Wallisville

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DRPK & WALV Measured vs Modeled

CB05-HR VOC (ETH, OLE & IOLE)

Deer Park

Wallisville

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Extended Model Performance Evaluation – TexAQS II Data
TexAQS II provides opportunities to examine model performance in unprecedented detail

- TexAQS II measurements allow us to examine model performance in places normally not reachable:
  - Additional stationary monitoring platforms:
    - Atop the Moody Tower
    - TexAQS II rural monitoring network
  - Mobile platforms:
    - Research Aircraft (four)
    - Research Vessel Ron Brown
    - Balloons
    - Instrumented Van (Solar Occultation Flux)
TexAQS II provides opportunities to examine model performance in unprecedented detail

- TexAQS II measurements allow us to examine model performance for chemical and physical processes not normally measured:
  - Measurements of a very large number of emitted species, intermediate reaction products, termination products, and reaction rates. Examples include:
    - Formaldehyde, nitric acid, HONO, photolysis rates, PAN compounds, assorted radicals, peroxides, various VOCs, etc. etc.
Why Is All This Important?

• Basic model performance for ozone just compares modeled concentrations with measurements. If they agree reasonably well, shouldn’t that be enough?

• No, because:
  – The model may reproduce observed ozone concentrations reasonably well, but may not correctly simulate the underlying chemical and physical processes – “Getting the Right Answer for the Wrong Reason”.

  – If we can assure ourselves that the model simulates these processes well, we will have more confidence that the model will respond correctly to changes in its inputs, specifically emissions growth and controls.
Some Aircraft Data Comparisons

- The NOAA P3 Orion flew missions in Houston and East Texas on 18 days between August 31 and October 13, 2006, collecting information on dozens of chemical species relevant to ozone production.

- The following slides provide a sample of the comparisons we have made to date.

- We are currently working on comparisons with data collected from other aircraft, the RV Ron Brown, Moody Tower, and other stationary and mobile sampling platforms.
9/13/06 P3 Measured & CAMx Modeled O₃ Mixing Ratios, full flight path
9/13/06 P3 Measured & CAMx Modeled O₃ Mixing Ratios inside the HG 2 Km Grid

Modeled and P3 Observed O₃ 09/13/2006

NOAA P3 Measured O₃ Mixing Ratio
09/13/2006

CAMx Reg8_PSCFV2 Modeled O₃ Mixing Ratio
09/13/2006
9/15/06 P3 Measured & CAMx Modeled O₃ Mixing Ratios, full flight path

Modeled and P3 Observed O₃ 09/15/2006

Reg8_PSCFV2 - Full P3 Flight Path

CAMx Reg8_PSCFV2 Modeled O₃ Mixing Ratio 09/15/2006
9/15/06 P3 Measured & CAMx Modeled O₃ Mixing Ratios inside the HG 2 Km Grid

Modeled and P3 Observed O₃ 09/15/2006

NOAA P3 Measured O₃ Mixing Ratio
09/15/2006

CAMx Reg8_PSCFV2 Modeled O₃ Mixing Ratio
09/15/2006

Observed Wind
5 m/sec.

Vertical Model Layer
4 Coarse Grid Lyr

NOx Point Source Locations

ppbv
9/13/06 P3 Measured & CAMx Modeled Formaldehyde Mixing Ratios, full flight path
9/13/06 P3 Measured & CAMx
Modeled Formaldehyde Mixing Ratios inside the HG 2 Km Grid

Modeled and P3 Observed FORM 09/13/2006

CAMx Reg8_PSCFV2 Modeled FORM Mixing Ratio
09/13/2006
9/15/06 P3 Measured & CAMx Modeled Formaldehyde Mixing Ratios, full flight path

Modeled and P3 Observed FORM 09/15/2006

NOAA P3 Measured FORM Mixing Ratio 09/15/2006

CAMx Reg8_PSCFV2 Modeled FORM Mixing Ratio 09/15/2006
9/15/06 P3 Measured & CAMx Modeled Formaldehyde Mixing Ratios inside the HG 2 Km Grid

NOAA P3 Measured FORM Mixing Ratio 09/15/2006

CAMx Reg8_PSCFV2 Modeled FORM Mixing Ratio 09/15/2006

Modeled and P3 Observed FORM 09/15/2006

Modeled and P3 Observed FORM 09/15/2006

Observed Wind

Vertical Model Layer

NOx Point Source Locations

Vertical Grid Layer
9/13/06 P3 Measured & CAMx Modeled Nitric Acid Mixing Ratios, full flight path

Modeled and P3 Observed HNO₃ 09/13/2006

![Modeled and P3 Observed HNO₃ 09/13/2006](image1)

NOAA P3 Measured HNO₃ Mixing Ratio
09/13/2006

![NOAA P3 Measured HNO₃ Mixing Ratio 09/13/2006](image2)

CAMx Reg8_PSCFV2 Modeled HNO₃ Mixing Ratio
09/13/2006

![CAMx Reg8_PSCFV2 Modeled HNO₃ Mixing Ratio 09/13/2006](image3)
9/13/06 P3 Measured & CAMx Modeled Nitric Acid Mixing Ratios inside the HG 2 Km Grid

NOAA P3 Measured HNO3 Mixing Ratio
09/13/2006

CAMx Reg8_PSCFV2 Modeled HNO3 Mixing Ratio
09/13/2006

Modeled and P3 Observed HNO3 09/13/2006
Reg8_PSCFV2 – Inside 2Km Grid

Modeled Wind
5 m/sec.

Vertical Layer
Coarse Grid Lyr
Fine Grid Lyr

Nox Point Source Locations
9/15/06 P3 Measured & CAMx Modeled Nitric Acid Mixing Ratios, full flight path

Modeled and P3 Observed HNO3 09/15/2006

NOAA P3 Measured HNO3 Mixing Ratio 09/15/2006

CAMx Reg8_PSCFV2 Modeled HNO3 Mixing Ratio 09/15/2006
9/15/06 P3 Measured & CAMx Modeled Nitric Acid Mixing Ratios inside the HG 2 Km Grid

Modeled and P3 Observed HNO3 09/15/2006

CAMx Reg8_PSCFV2 Modeled HNO3 Mixing Ratio 09/15/2006

Observed Wind

Vertical Model Layer

NOx Point Source Locations

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