Proximate Modeling of Weekend Ozone - Results for Several Hypotheses and Years

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Presented by
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Sponsors and Participants

• **Coordinating Research Council**

• **US DOE Office of Heavy Vehicle Technologies**
  Dr. Michael Gurevich, Program Manager
  – Funded through the National Renewable Energy Laboratory

• **Participants**
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  – AIR: Jon Heuss, Jeremy Heiken
Presentation Outline

• Recap of October 2001 Presentation
• New Results
  – Friday Changes in MV Emissions and Carryover
  – Spatial Shift in MV Emissions
  – Aerosol Impact on Photolysis Rates
  – Weekend Effect in 1987 and 2010
  – SAPRC99 Chemical Mechanism
• Summary
October 2001 Presentation

• Described methods, models and databases
• Results for NOx Mass and Timing Hypotheses
  – looked at Saturday/Sunday changes in MV emissions for 1997
  – timing effect small compared to mass effect
  – modeled effects strikingly similar to observed effects for ozone and precursors

• http://www.arb.ca.gov/aqd/weekendeffect/weekendeffect.htm
Observed WE Effect at Azusa for Comparison with Later Model Results

Azusa, Summer 1995

O3 Accumulation
\[ t = \frac{t_{O3_{max}} - t_{NO=O3}}{t_{NO=O3}} \]

Post Maximum O3
Declining photolysis rate, increasing mixing and ventilation, and titration of O3 by fresh NO emissions

O3 Inhibition
(due to NO titration)

Carry Over
O3, NO2, and PAN
HONO and HCHO
NO, CO, and VOC

Post Maximum O3
Declining photolysis rate, increasing mixing and ventilation, and titration of O3 by fresh NO emissions

 Carry Over
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Post Maximum O3
Declining photolysis rate, increasing mixing and ventilation, and titration of O3 by fresh NO emissions

O3 Inhibition
(due to NO titration)

Hour (PDT)

O3, NO and NO2* (ppm)

WE O3
WD O3
WE NO
WD NO
WE NO2*
WD NO2*
WE CO
WD CO

O3 Inhibition
(due to NO titration)

WE O3
WD O3
WE NO
WD NO
WE NO2*
WD NO2*
WE CO
WD CO

a. O3 accumulation rate = \[O3_{(max)} - O3_{(NO=O3)}]/(t_{O3_{max}} - t_{NO=O3})\]

* Figure courtesy of Eric Fujita, DRI.
http://www.arb.ca.gov/aqd/weekendeffect/nre1p1v1f.pdf

Presents:slides/greg/A36Awdwe_022002a.ppt
Azusa: Change Mass and Temporal Profile of MV Emissions

Ozone and Precursors at Azusa
# Model Run “Cheat Sheet”

<table>
<thead>
<tr>
<th>Run Number</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>wd_base</td>
<td>August 3-7, 1997 with every day as a weekday</td>
</tr>
<tr>
<td>wd_base_s99</td>
<td>wd_base using SAPRC99</td>
</tr>
<tr>
<td>h1a</td>
<td>change MV mass on Sat/Sun based on activity data</td>
</tr>
<tr>
<td>h1b</td>
<td>h1a using SAPRC99</td>
</tr>
<tr>
<td>h2a</td>
<td>change MV temporal profile on Sat/Sun based on activity data</td>
</tr>
<tr>
<td>h2c</td>
<td>change MV mass and temporal profile on Sat/Sun</td>
</tr>
<tr>
<td>h2d</td>
<td>h2c using SAPRC99</td>
</tr>
<tr>
<td>h2e</td>
<td>h3a plus h2f – change Fri/Sat/Sun MV mass/temporal/spatial</td>
</tr>
<tr>
<td>h2f</td>
<td>change MV spatial distribution on Fri/Sat/Sun</td>
</tr>
<tr>
<td>h3a</td>
<td>h2c plus Friday MV mass and temporal profile change</td>
</tr>
<tr>
<td>h3b</td>
<td>wd_base plus Friday MV mass and temporal profile change</td>
</tr>
<tr>
<td>h4a</td>
<td>h2c changing Sunday only</td>
</tr>
<tr>
<td>h5a</td>
<td>change photolysis rates on Sat/Sun to reflect lower aerosol load</td>
</tr>
</tbody>
</table>
Friday Emission Change and Carryover

- Change mass and timing of Friday MV emissions based on activity data
- Little impact on daily maximum ozone on Friday or Saturday

**Change Friday MV – Friday Impact (run=h3b)**

CRC Proximate Modeling – Change in Daily Max Ozone (ppb)

**Change Friday MV – Saturday Impact (run=h3b)**

CRC Proximate Modeling – Change in Daily Max Ozone (ppb)
Friday through Monday Carryover at Azusa

- Carryover is small relative to same day effect of Saturday and Sunday emissions changes
Weekend Spatial Shift in MV Emissions

• **Hypothesis:** less commute, more local driving on weekend

• **Proximate representation**
  – NREL sponsored STI analysis of day of week differences in WIM data at 8 locations for LDV and HDV
  – ENVIRON gridded the differences by Kriging
  – Spatially shift the MV emissions while conserving total mass

• **Resulting spatial shift crudely approximates hypothesis**

• **Suitable for proximate modeling**

• **Not intended to represent reality**
Saturday Emissions Shift

Grey areas have low or zero MV emissions

* Vehicle count data courtesy of Lyle Chinkin, STI
Saturday Effect of MV Emissions Shift

- Increases in daily maximum ozone through most of the basin
- Pattern of increases similar to MV mass/timing change
- Spatial shift and mass/timing changes are roughly additive
Aerosol Impact on Photolysis Rates and Ozone

- Hypothesis: lower aerosol load on weekend increases photolysis rates and accelerates ozone formation
- Measured optical depths due to aerosols at Riverside in summer 1997 were in range 1.0 to 0.2 at 340 nm: LLNL/UC Berkeley/Envair report for ARB (96-335)
- No data on WD/WE differences. Therefore, model the maximum range (0.2 to 1.0) to test sensitivity
- Changing CAMx Photolysis rates
  - CAMx uses the TUV radiation model from NCAR
  - LLNL/UCB report for ARB also used TUV, but with less accurate numerics than CAMx uses ("2-stream" rather than "discrete ordinates")
Photolysis Rate Sensitivity

NO2 photolysis rate for an aerosol optical depth of 1.0 relative to 0.2

Zenith angle vs. j(NO2) Ratio (j(NO2) surface, j(NO2) 640 m, j(NO2) 1840 m)
Air Quality Sensitivity to Aerosols

- Results inconsistent with aerosols being important cause of weekend effect
  - Almost no changes in precursor concentrations
  - Ozone changes too small and have wrong temporal profile

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**Decrease Aerosol Loading (run=h5a)**

CRC Proximate Modeling - Surface Ozone Change (ppb)
Photolysis Rate Impact of Reducing Aerosol O.3. from 1.0 to 0.2

**Aerosol Impact via Photolysis Rates at Azusa (run=h5a)**

- O3 - High Aerosol
- O3 - Low Aerosol
- NO - High Aerosol
- NO - Low Aerosol
- NO2 - High Aerosol
- NO2 - Low Aerosol
- VOC - High Aerosol
- VOC - Low Aerosol

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Weekend Effect in 1987 and 2010

- Keep meteorology and biogenic emissions the same
- 1987 anthropogenic emissions from ARB for Aug 28, 1987
- 2010 anthropogenic emissions from SCAQMD
  - Based on August 28, 1987 SCAQS
  - EMFAC2000
  - Includes advanced technology controls (black box)
  - Consistency with ARB 87 and 97 emissions?
- Model a weekday base case and Fri/Sat/Sun change to MV mass and temporal profiles
Emissions for 1987, 1997 and 2010

Emission Totals for the SCAQS Domain
2010 Emissions Projections Are Uncertain

- Future year inventories inherit uncertainties from base year inventories

- Future year emissions projections contain additional uncertainties from assumed activity growth and control strategy effectiveness
Peak Ozone for Aug 5 in 1987/1997/2010

1997 Base Case (run=wd_base)
CRC Proximate Modeling – Daily Max Ozone (ppb)

1987 Base Case (run=87_wd_base)
CRC Proximate Modeling – Daily Max Ozone (ppb)

2010 Base Case (run=10_wd_base)
CRC Proximate Modeling – Daily Max Ozone (ppb)
Saturday Effect on Ozone

Change MV Mass & Temporal in 1997

CRC Proximate Modeling – Change in Daily Max Ozone (ppb)

Change MV Mass & Temporal in 1987

CRC Proximate Modeling – Change in Daily Max Ozone (ppb)

Change MV Mass & Temporal in 2010

CRC Proximate Modeling – Change in Daily Max Ozone (ppb)
Comparison Across Years

- 1987 has higher ozone than 1997 and generally similar weekend ozone effect
- 2010 has lower ozone than 1997
- 2010 weekend effect shows smaller area of weekend ozone increase and larger area of no change or decrease
- Results for 2010 are based on the emissions reductions included in the current Los Angeles AQMP
Effects at Azusa in 2010

- Weekend ozone effect is smaller in 2010 than 1997
- 2010 “signature” is similar to 1997
  - higher morning VOC/NOx ratio on weekends
  - higher weekend ozone in morning through midday

Change MV Mass and Timing: 1997 Effect at Azusa (run=h3a)

Change MV Mass and Timing: 2010 Effect at Azusa (run=10_h3a)
SAPRC99 Mechanism Sensitivity

- SAPRC99 mechanism in CAMx version 3.1
  - fixed parameter version also used in CMAQ
- ARB emissions available for SAPRC99 and CB4
- Impact on modeling results
  - Model performance evaluation
  - Weekend effect for scenario h2c - change MV mass and temporal profiles for Sat/Sun in 1997
Higher Ozone with SAPRC99

- Daily maximum ozone for August 6, 1997. Other days show similar differences between CB4 and SAPRC99
Poor Model Performance with SAPRC99

Comparison of CAMx/MM5 1-hour ozone model performance statistics with CB4 and SAPRC99 emissions. Gray shaded values fail the performance goal.

<table>
<thead>
<tr>
<th></th>
<th>EPA Goal</th>
<th>5-Aug</th>
<th>6-Aug</th>
<th>7-Aug</th>
</tr>
</thead>
<tbody>
<tr>
<td>Observed Peak (ppb)</td>
<td></td>
<td>187</td>
<td>154</td>
<td>150</td>
</tr>
<tr>
<td>CB4 Emissions</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Modeled Peak (ppb)</td>
<td></td>
<td>166.6</td>
<td>176.4</td>
<td>159</td>
</tr>
<tr>
<td>Unpaired Peak (%)</td>
<td></td>
<td>≤ ±20</td>
<td>-11</td>
<td>15</td>
</tr>
<tr>
<td>Normalized Bias (%)</td>
<td></td>
<td>≤ ±15</td>
<td>5</td>
<td>7</td>
</tr>
<tr>
<td>Normalized Error (%)</td>
<td></td>
<td>≤ 35</td>
<td>22</td>
<td>24</td>
</tr>
<tr>
<td>SAPRC99 Emissions</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Modeled Peak (ppb)</td>
<td></td>
<td>203.9</td>
<td>223.0</td>
<td>200.4</td>
</tr>
<tr>
<td>Unpaired Peak (%)</td>
<td></td>
<td>≤ ±20</td>
<td>9</td>
<td>45</td>
</tr>
<tr>
<td>Normalized Bias (%)</td>
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<td>≤ ±15</td>
<td>30</td>
<td>35</td>
</tr>
<tr>
<td>Normalized Error (%)</td>
<td></td>
<td>≤ 35</td>
<td>39</td>
<td>44</td>
</tr>
</tbody>
</table>

Statistical measures were calculated for valid data pairs with observed values > 60 ppb at 48 stations.
Weekend Effect with CB4 and SAPRC99

CB4 – Change MV – Saturday Impact (run=h2c)

SAP99 – Change MV – Saturday Impact (run=h2d)

CB4 – Change MV – Sunday Impact (run=h2c)

SAP99 – Change MV – Sunday Impact (run=h2d)
SAPRC99 Weekend Effect for Azusa

SAPRC99 Sat/Sun MV Mass/Timing Effect at Azusa (run=h2d)

- **O3-WE**
- **O3-WD**
- **NO-WE**
- **NO-WD**
- **NO2-WE**
- **NO2-WD**
- **VOC-WE**
- **VOC-WD**

**Graph Details:**
- X-axis: Hour (PST)
- Y-axis: O3, NO, NO2 (ppb)
- Y-axis: VOC (ppbC)

**Legend:**
- O3: Green dashed line
- NO: Blue solid line
- NO2: Orange solid line
- VOC: Green solid line

**Timeline:**
- 00:00 to 24:00

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SAPRC99 Findings

- Substantially higher ozone than CB4
- Poor base case model performance
- Response to weekend MV emission changes in poorer agreement with observations for downwind locations
- Response to weekend MV emission changes consistent with observations at Azusa
- SAPRC99 might perform well with different base emissions, e.g., less VOCs or more NOx
Conclusions on the Weekend Effect for Ozone

Proximate modeling results are consistent with the following conclusions

• Changes to the mass of onroad MV emissions on weekend days are the main cause of the weekend effect
• Changes to the spatial distribution of MV emissions on the weekend could contribute
• Weekend ozone is relatively insensitive to changes in the timing of MV emissions
Conclusions on the Weekend Effect for Ozone
(concluded)

• There is little carryover of effects from one weekend day to the next
• Changes in photolysis rates due to changes in aerosol load are not the cause of the weekend effect
• Based on the projected 2010 emissions in the current AQMP, the weekend effect for ozone will decrease in magnitude and extent by 2010