Characterization of Gulf Background Ozone Concentrations

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Purpose

- One of the perplexing model performance issues is the frequent over-prediction of ozone concentrations in air arriving from the Gulf.
- This work attempts to characterize the air masses arriving at a near-shore site (Galveston 99th Street Pier, C-1034) by calculating back-trajectories, associating each with observed Galveston ozone levels, and finally using a clustering algorithm to characterize groups of like trajectories.
Observed and Modeled Galveston Ozone Concentrations, June 2006

Wind Dir deg

Galveston Airport C34/A109/X152

$O_x (O_3+NO_x)$ Concentration (ppb) at Layer 1 (20060531-20060702)

GALC at (209.7,-1189.9) km (481670014, C34, Galveston Airport C34/A109/X152, 8715 Cessna Street, Galveston, Galveston Co., TX)
Observed and Modeled Galveston Ozone Concentrations, June 2006

Galveston Airport C34/A109/X152

O\textsubscript{x} (O\textsubscript{3}+NO\textsubscript{x}) Concentration (ppb) at Layer 1 (20060531-20060702)

GALC at (209.7,-1189.9) km (481670014, C34, Galveston Airport C34 A109/X152, 8715 Cessna Street, Galveston, Galveston Co., TX)
Methodology

- Back trajectories for five ozone seasons: May-September, 2007-11
- Endpoint was the Galveston 99th Street Pier monitor, C-1034
- Hybrid Single Particle Lagrangian Integrated Trajectory (HySPLIT) Model:
  - EDAS-40 km Meteorological data set
  - Termination at 100 M
  - 48 Hour trajectory length
  - End hours: 1, 3, 5, 7, 9, 11, 13, 15, 17, 19, 21 and 23
- Total of 8,792 trajectories
Methodology

- Next, each trajectory point was assigned the value of the ozone concentration monitored in Galveston at the time it arrived there.
- A 36x36 km grid was overlaid across the trajectory field and the terminal ozone concentrations of trajectory points falling in each grid cell was tabulated.
- For grid cells with enough (10+) trajectory points, cell median values were color-coded on top of the trajectories.
Galveston 48-Hour 100 M Back Trajectories
May-Sep, 2007-11
Minimum 10 Values per Grid Cell
Methodology

• To further study the trajectories, a clustering algorithm was used to find groups of similar clusters. This analysis included the vertical component of each trajectory point.

• Each trajectory was characterized as a 144-dimensional vector \((X_1-X_{48}, Y_1-Y_{48}, Z_1-Z_{48})\), then normalized to give each of the 144 components equal weight.
Methodology

- The SAS FASTCLUS procedure was used to define 8 clusters of back trajectories.

```sas
Proc Standard Data=Trajedy Out=Stand Mean=0 Std=1;
Var X1-X48 Y1-Y48 Z1-Z48;
Proc FastClus Noprint Data=Stand Out=Clust MaxClusters=8;
Var X1-X48 Y1-Y48 Z1-Z48;
Run;
```

- A color coding scheme like that used earlier for the full set of trajectories was employed for each cluster.
Cluster 1 Back Trajectories
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11
**Cluster 1 Median Terminal Ozone Concentrations**

Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11

Minimum 10 Values per Grid Cell

Cluster 1: 104 Trajectories

Terminal Ozone Concentrations:
- 10\textsuperscript{th} Percentile: 20 ppb
- Median: 34 ppb
- 90\textsuperscript{th} Percentile: 49 ppb
Cluster 2 Back Trajectories
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11
Cluster 2 Median Terminal Ozone Concentrations
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11

Minimum 10 Values per Grid Cell

Cluster 2: 417 Trajectories
Terminal Ozone Concentrations:
10th Percentile 13 ppb
Median 24 ppb
90th Percentile 49 ppb
Cluster 3 Back Trajectories
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11

Cluster 3 10th, 50th, and 90th Percentile Trajectory Elevations

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Cluster 3 Median Terminal Ozone Concentrations
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11

Minimum 10 Values per Grid Cell

Cluster 3: 11 Trajectories
Terminal Ozone Concentrations:
10th Percentile 16 ppb
Median 18 ppb
90th Percentile 24 ppb
Cluster 4 Back Trajectories
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11
Cluster 4 Median Terminal Ozone Concentrations

Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11

Minimum 10 Values per Grid Cell

Cluster 4: 1095 Trajectories
Terminal Ozone Concentrations:
10th Percentile 17 ppb
Median 26 ppb
90th Percentile 44 ppb
Cluster 5 Back Trajectories
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11
Cluster 5 Median Terminal Ozone Concentrations
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11

Minimum 10 Values per Grid Cell

Cluster 5: 1058 Trajectories
Terminal Ozone Concentrations:
10th Percentile    20 ppb
Median             46 ppb
90th Percentile   69 ppb
Cluster 6 Back Trajectories
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11
Cluster 6 Median Terminal Ozone Concentrations
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11

Minimum 10 Values per Grid Cell

Cluster 6: 8 Trajectories
Terminal Ozone Concentrations:
10th Percentile       6 ppb
Median                19.5 ppb
90th Percentile      26 ppb
Cluster 7 Back Trajectories
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11
Cluster 7 Median Terminal Ozone Concentrations
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11

Minimum 10 Values per Grid Cell

Cluster 7: 3638 Trajectories
Terminal Ozone Concentrations:
10th Percentile  14 ppb
Median           21 ppb
90th Percentile  45 ppb
Cluster 8 Back Trajectories
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11
Cluster 8 Median Terminal Ozone Concentrations
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11
Minimum 10 Values per Grid Cell

Cluster 8: 104 Trajectories
Terminal Ozone Concentrations:
10th Percentile 16 ppb
Median 21 ppb
90th Percentile 42 ppb
Cluster 1 Median Terminal Ozone Concentrations
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11
Minimum 10 values per Grid Cell

104 Trajectories
10th Percentile O3 20 ppb
Median O3 34 ppb
90th Percentile O3 49 ppb

Cluster 2 Median Terminal Ozone Concentrations
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11
Minimum 10 values per Grid Cell

417 Trajectories
10th Percentile O3 13 ppb
Median O3 24 ppb
90th Percentile O3 49 ppb

Cluster 3 Median Terminal Ozone Concentrations
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11
Minimum 10 values per Grid Cell

1095 Trajectories
10th Percentile O3 17 ppb
Median O3 26 ppb
90th Percentile O3 44 ppb

Cluster 4 Median Terminal Ozone Concentrations
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11
Minimum 10 values per Grid Cell

1058 Trajectories
10th Percentile O3 20 ppb
Median O3 46 ppb
90th Percentile O3 69 ppb

Cluster 5 Median Terminal Ozone Concentrations
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11
Minimum 10 values per Grid Cell

3638 Trajectories
10th Percentile O3 14 ppb
Median O3 21 ppb
90th Percentile O3 45 ppb

Cluster 7 Median Terminal Ozone Concentrations
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11
Minimum 10 values per Grid Cell

104 Trajectories
10th Percentile O3 16 ppb
Median O3 21 ppb
90th Percentile O3 45 ppb

Cluster 8 Median Terminal Ozone Concentrations
Galveston 48-Hour 100 M Back Trajectories, May-Sep, 2007-11
Minimum 10 values per Grid Cell

104 Trajectories
10th Percentile O3 16 ppb
Median O3 21 ppb
90th Percentile O3 45 ppb
Conclusions

- Associating back-trajectories with terminal ozone concentrations provides an intuitive means for understanding the origins of transported ozone.

- Clustering the trajectories helps to further identify sources of high and low background, and provides insight into the vertical component of the transport path.
Conclusions

- The lowest ozone concentrations are associated with trajectories that remained over the central Gulf for at least 48 hours.
- Higher concentrations are associated with trajectories that pass close to the northern and western Gulf Coast.
- The highest concentrations are associated with trajectories that remain primarily over land.
Acknowledgement

- Thanks to Fernando Mercado for mass-producing the HySPLIT trajectories used in this analysis.