Characterization of Gulf of Mexico Background Ozone Concentrations

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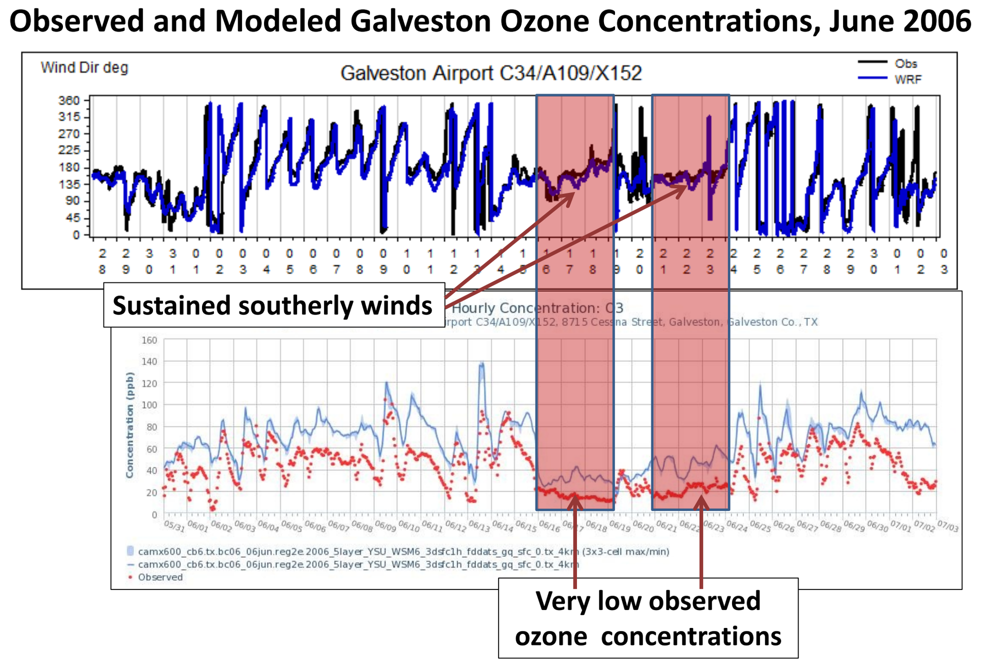
Abstract

A perplexing problem with model performance in the Houston/Galveston area is the frequent over-prediction of ozone concentrations in air arriving from the Gulf of Mexico.

Examination of three-dimensional back-trajectories helps to identify the origins of very clean air often seen at coastal sites in Texas. This work attempts to characterize the air masses arriving at near-shore sites on the Texas coast by calculating three-dimensional back-trajectories, associating each with observed ozone concentrations at the trajectory's terminus, and finally using a clustering algorithm to characterize groups of like trajectories. Color-coding the trajectories according to the ozone concentrations at the terminus provides a highly intuitive approach to characterizing the sources of background ozone.

Observed and Modeled Galveston Ozone Concentrations, June 2006



Methodology

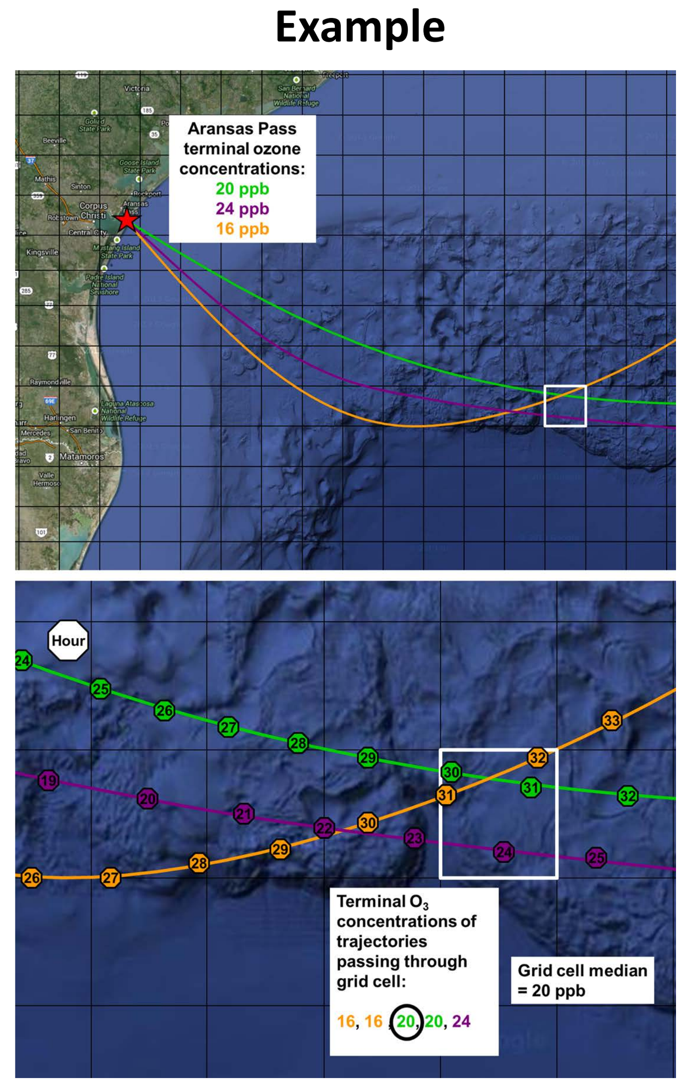
- Back-trajectories for five ozone seasons were developed: May-September, 2007 through 2011.
- Endpoints were at monitors in Galveston, Sabine Pass, and Aransas Pass.
- Hybrid Single Particle Lagrangian Integrated Trajectory (HySPLIT) Model:
  - EDAS-40 km Meteorological data set
  - Termination at 100 M
  - 48 Hour trajectory length
  - End hours: 1,3,5,7,9,11,13,15,17,19,21 and 23
- To further study the trajectories, a clustering algorithm was used to find groups of similar clusters. This analysis included the log-transformed 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.
- Next, each trajectory point was assigned the value of the observed ozone concentration at the time it arrived at the monitor.
- 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 (30+) trajectory points, cell median values were calculated and the grid cells were color-coded on top of the trajectories.
- The SAS FASTCLUS procedure was used to define clusters of back trajectories.

```
Data Traj; Set In.Merged_&MSite;
  Array Alt(48) Alt1-Alt48; Array LA(48) LA1-LA48;
   Do hour=1 to 48;
      LA(Hour) = Log(Max(Alt(Hour),1));
   End;
   Drop hour;
Proc STDIZE Data=Traj out=Stand; Var X1-X48 Y1-Y48 LA1-LA48;
Proc FASTCLUS Summary Data=Stand Out=Clust MaxClusters=10 Maxiter=1000
   Drift   Delete=200  Converge=.0001  Radius=15 Strict=17;
  Var X1-X48 Y1-Y48 LA1-LA48;
Run;
```

- A color coding scheme like that used for the full set of trajectories was employed for each cluster (minimum 15 trajectory points per grid cell).

Monitor Locations

Example



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.
- 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.

Notes: The technique used here to produce the color-coded tile plots is based on the Potential Source Contribution Function (PSCF) approach [Ashbaugh, *et al* (1985), Hopke (2003), Xie and Berkowitz (2006)]. This approach was used by the TCEQ to reconcile observed concentrations of certain highly-reactive Volatile Organic Compounds (HRVOCs) with reported inventories in the Houston-Galveston area [TCEQ (2010)].

References:

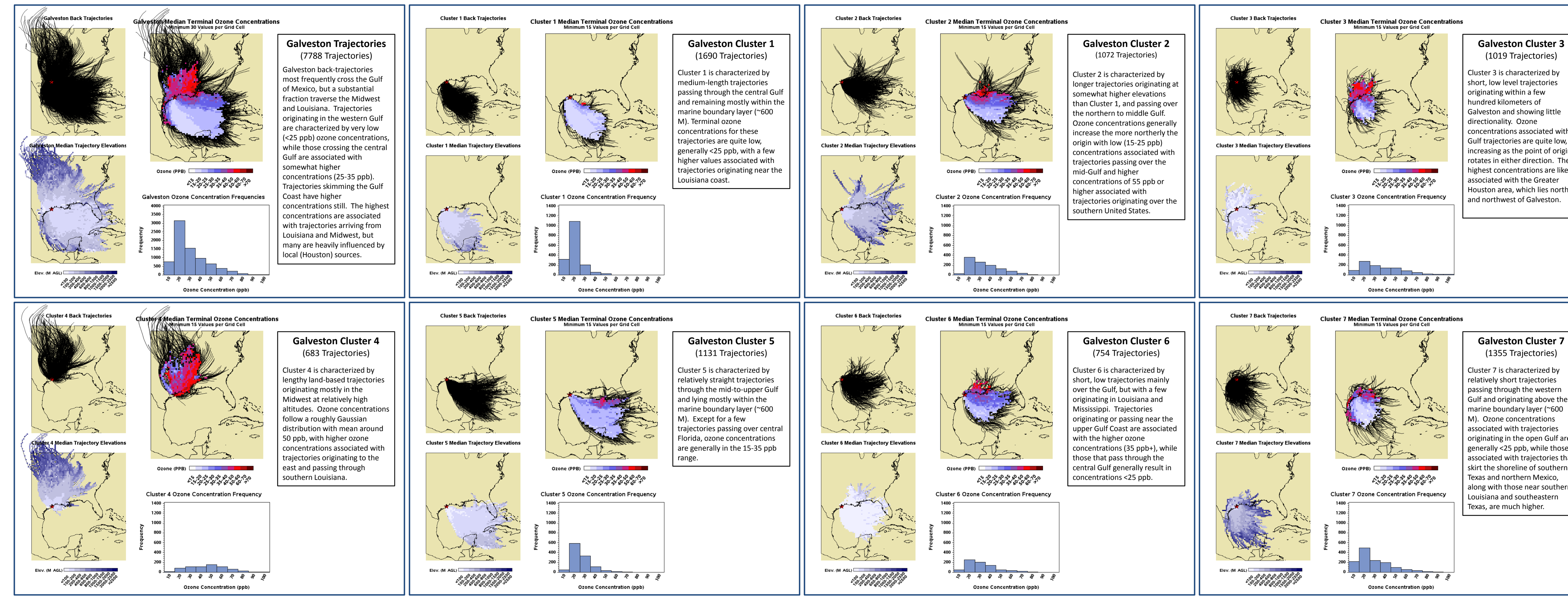
Ashbaugh, L.L., Malm, W.C., Sadeh, W.Z., (1985). A residence time probability analysis of sulfur concentrations at Grand Canyon National Park. Atmospheric Environment 19 (8), 1263–1270.

Hopke, P.K., (2003). Recent development in receptor modeling. Journal of Chemometrics 17, 1–12.

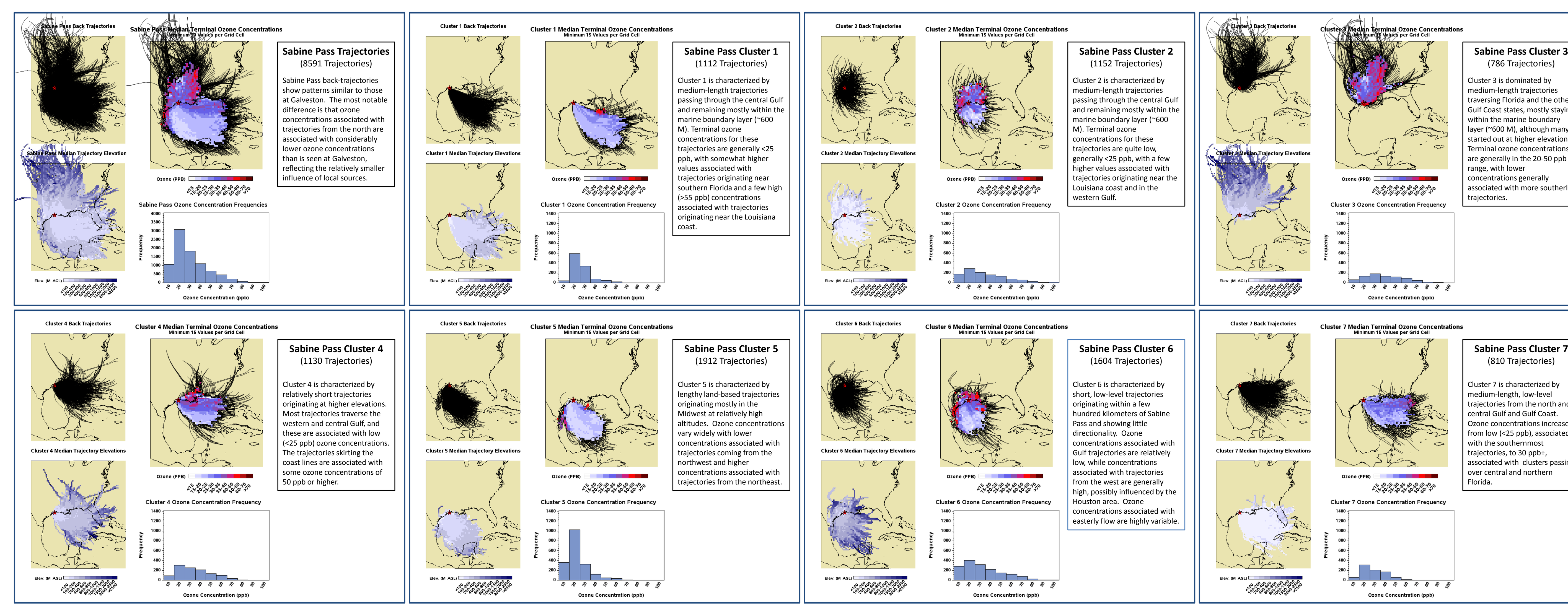
Xie Yulong and Berkowitz, Carl M. (2007), The use of conditional probability functions and potential source contribution functions to identify source regions and advection pathways of hydrocarbon emissions in Houston, Texas, Atmospheric Environment 41 (2007) 5831–5847.

TCEQ, Houston-Galveston-Brazoria Attainment Demonstration State Implementation Plan Revision for the 1997 Eight-Hour Ozone Standard, March, 2010.

Galveston (7 Clusters)



Sabine Pass (7 Clusters)



Aransas Pass (6 Clusters)