

The Influence of Air Toxics Emissions Inventory Selection on Air Quality Model Predictions in Corpus Christi, Texas

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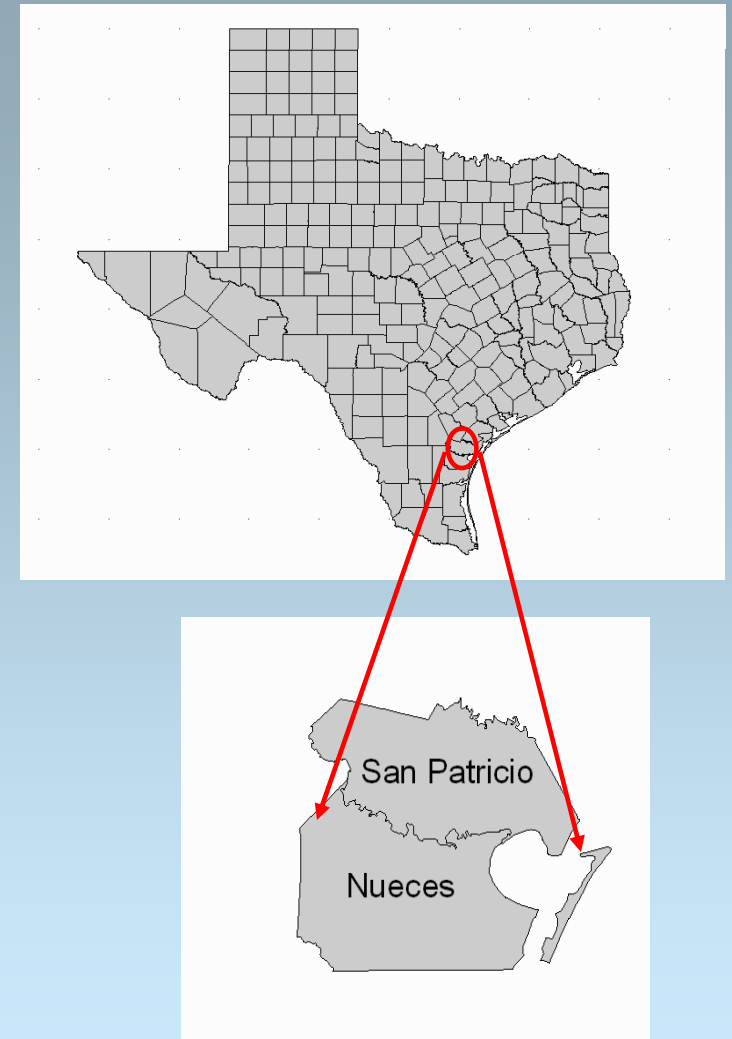
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Background: Corpus Christi

- Population of 400,000 in Nueces and San Patricio Counties.
- The Port of Corpus Christi in Nueces County includes a significant petroleum refining and chemical manufacturing complex in close proximity to residential areas.
- Many air toxics are ozone precursors.



Corpus Christi Air Monitoring and Surveillance Camera Installation and Operation Project

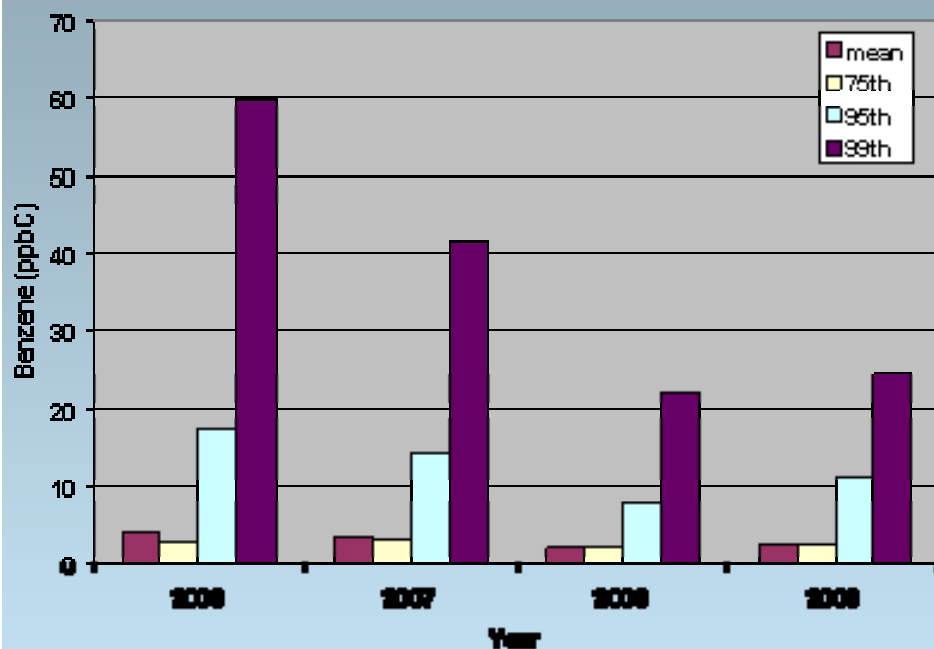


- Sulfur compounds, TNMHC, and meteorological measurements at all seven UT sites since June 2005.

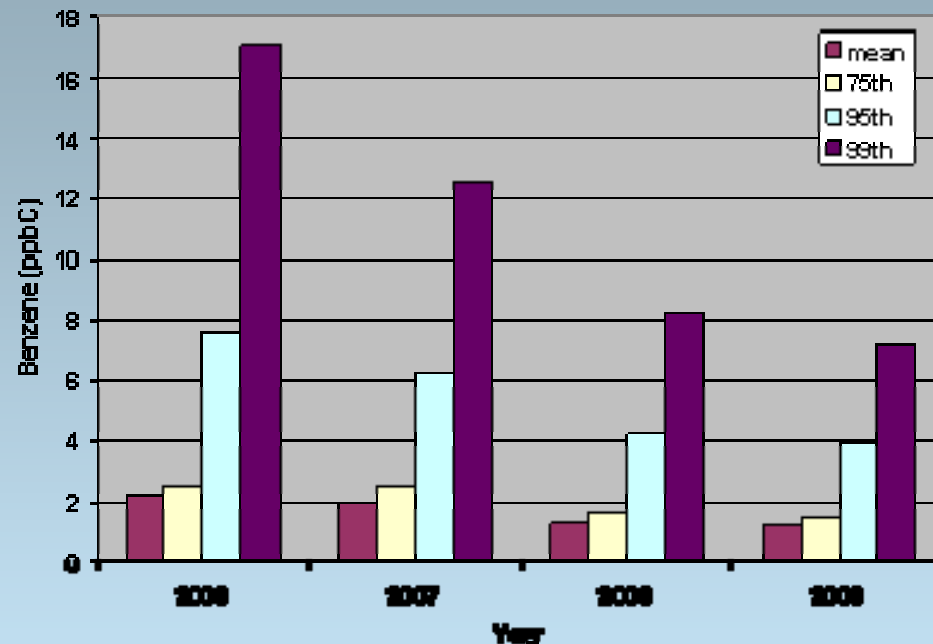
- Hourly auto-GC measurements and camera surveillance at two sites (Oak Park and Solar Estates in blue above).

- Event triggered canisters at five sites ($\text{TNMHC} \geq 2000 \text{ ppbC}$ for 15 min).

Measured Benzene Concentrations at Oak Park and Solar Estates Auto-GC Sites: 2006-2009



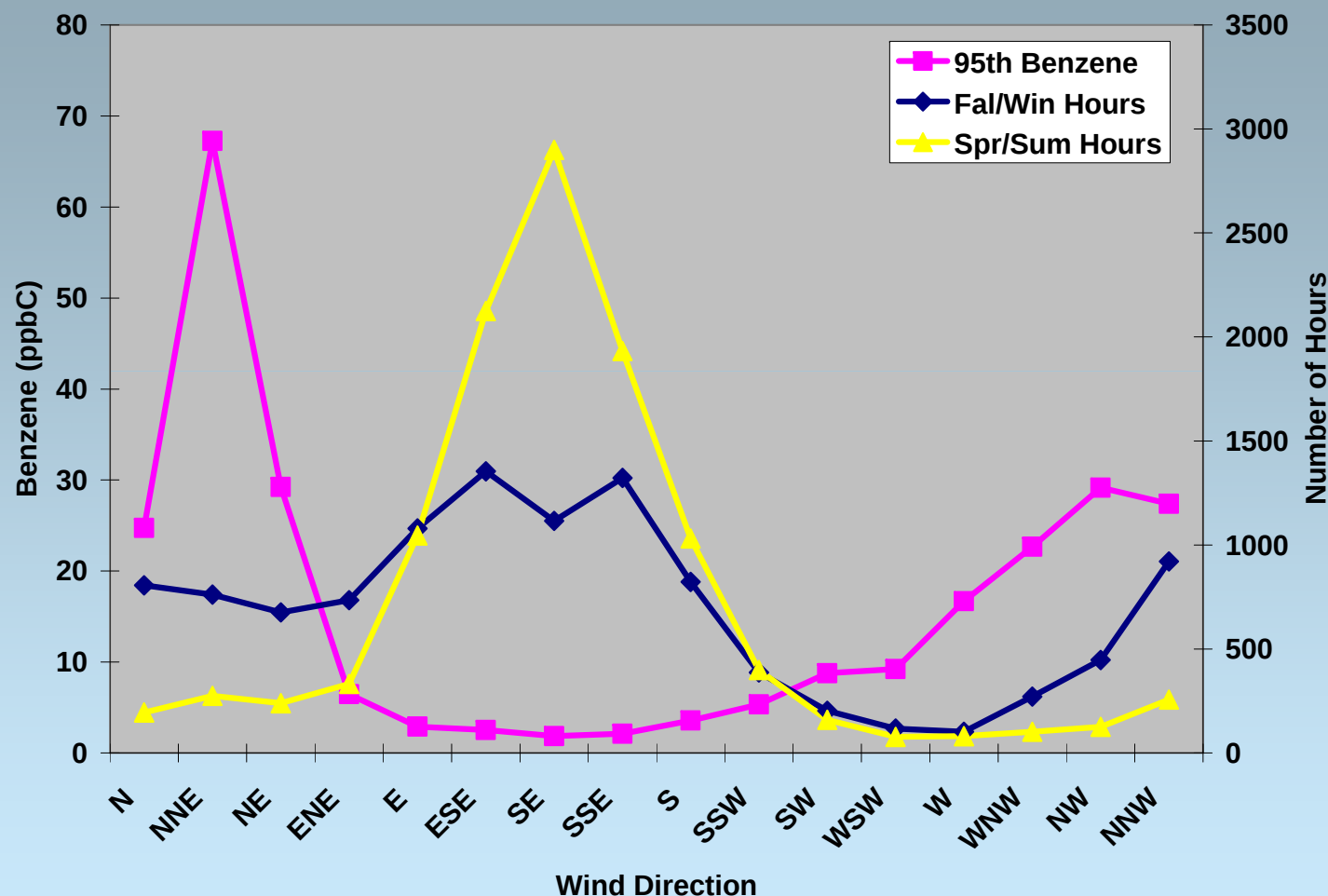
Oak Park



Solar Estates

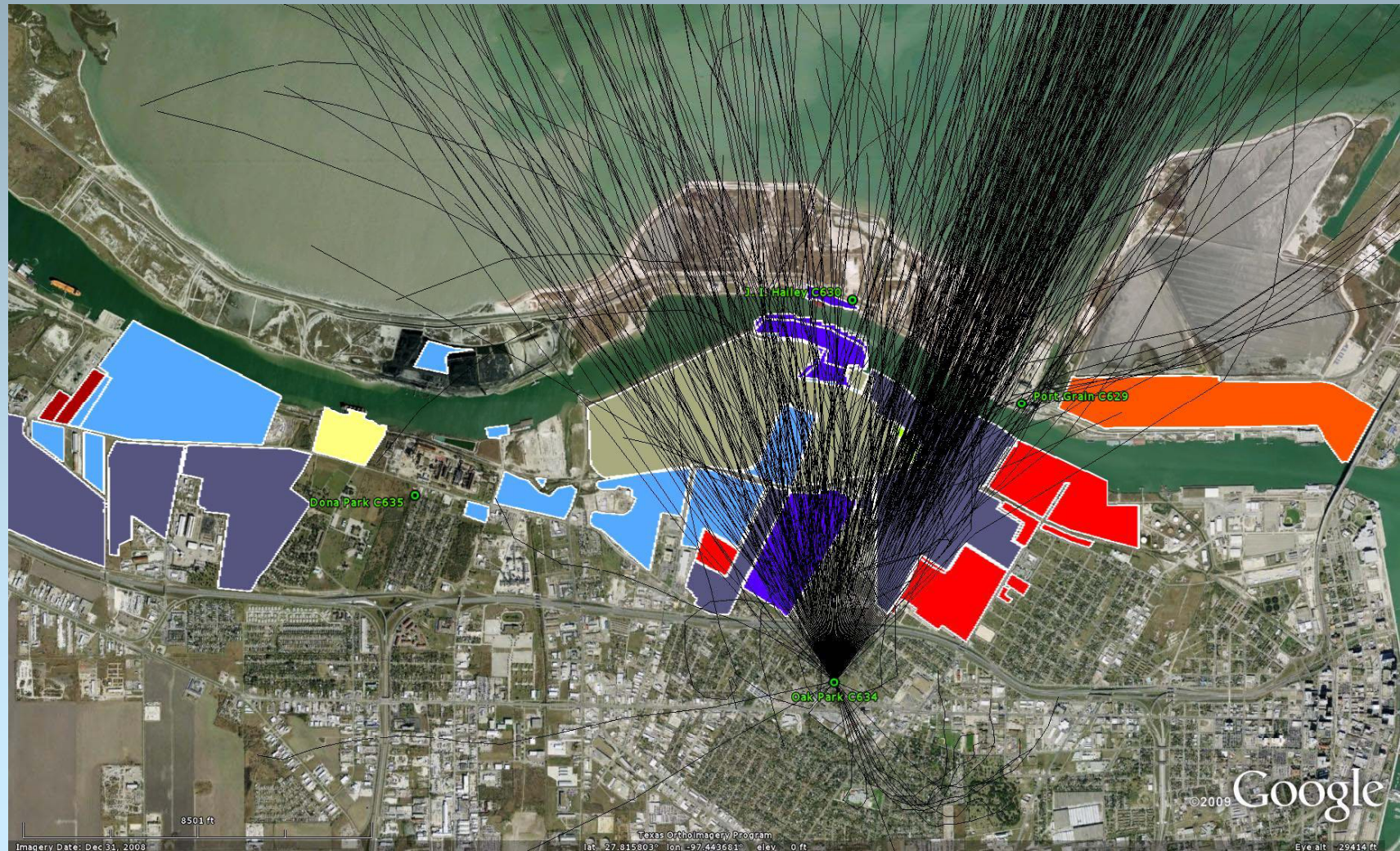
- Benzene concentrations at Oak Park are higher than at Solar Estates (note differences in scales).
- U.S. EPA's Toxics Release Inventories also show decreases in benzene emissions between 2005-2008.

Observed Benzene Concentrations at Oak Park and Wind Direction Frequency during 2006 – 2008

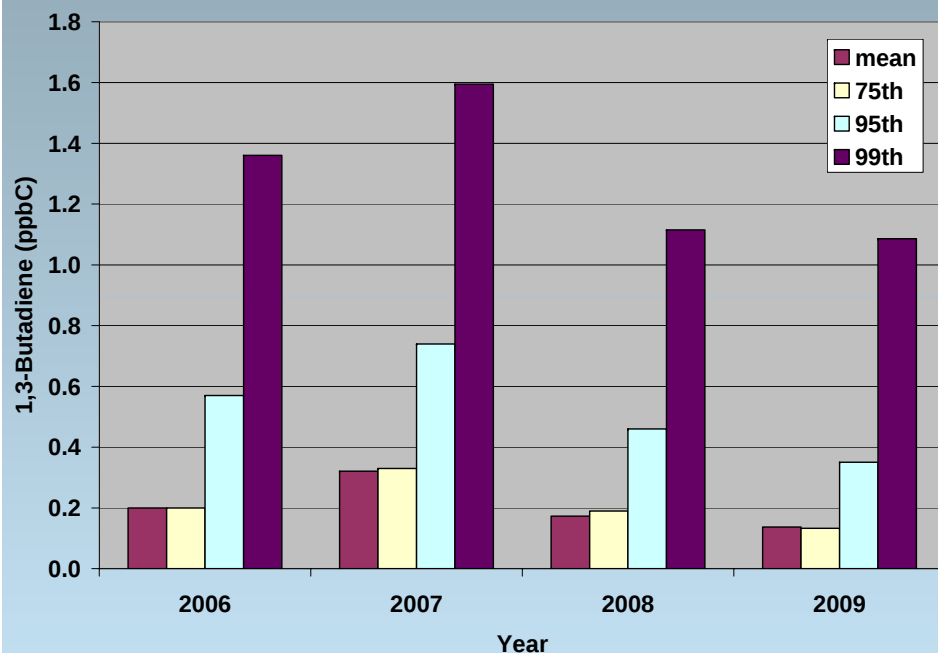


- Frequency of wind directions associated with higher benzene concentrations (i.e., north-northwest or north-northeast) is greater during the Fall/Winter than Spring/Summer.

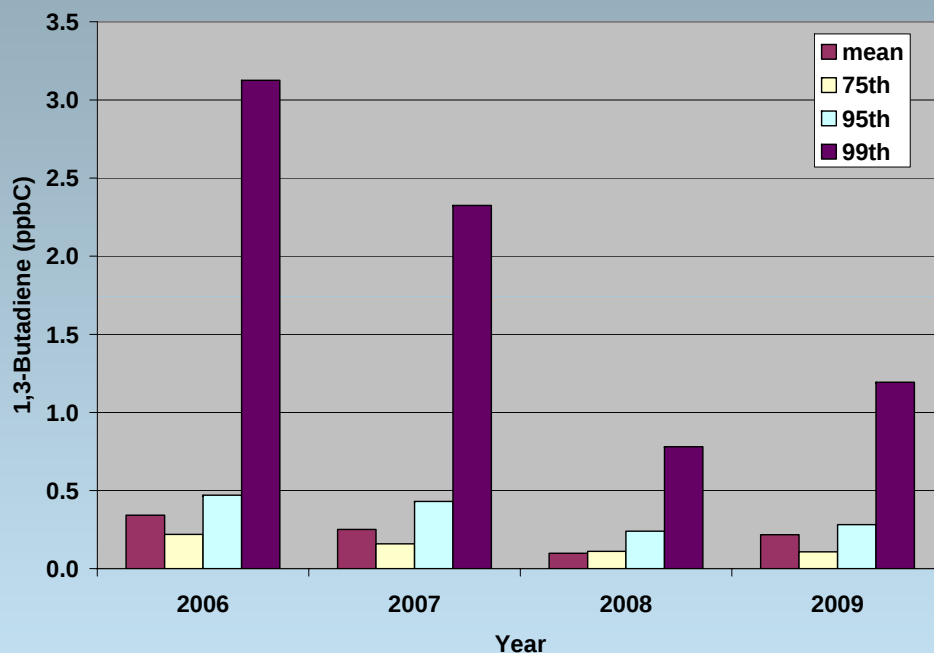
Upwind Source Regions when Benzene Concentrations are 30 ppbC or Greater at Oak Park Based on Surface Wind Back Trajectories



Measured 1,3-Butadiene Concentrations at Oak Park and Solar Estates Auto-GC Sites: 2006-2009



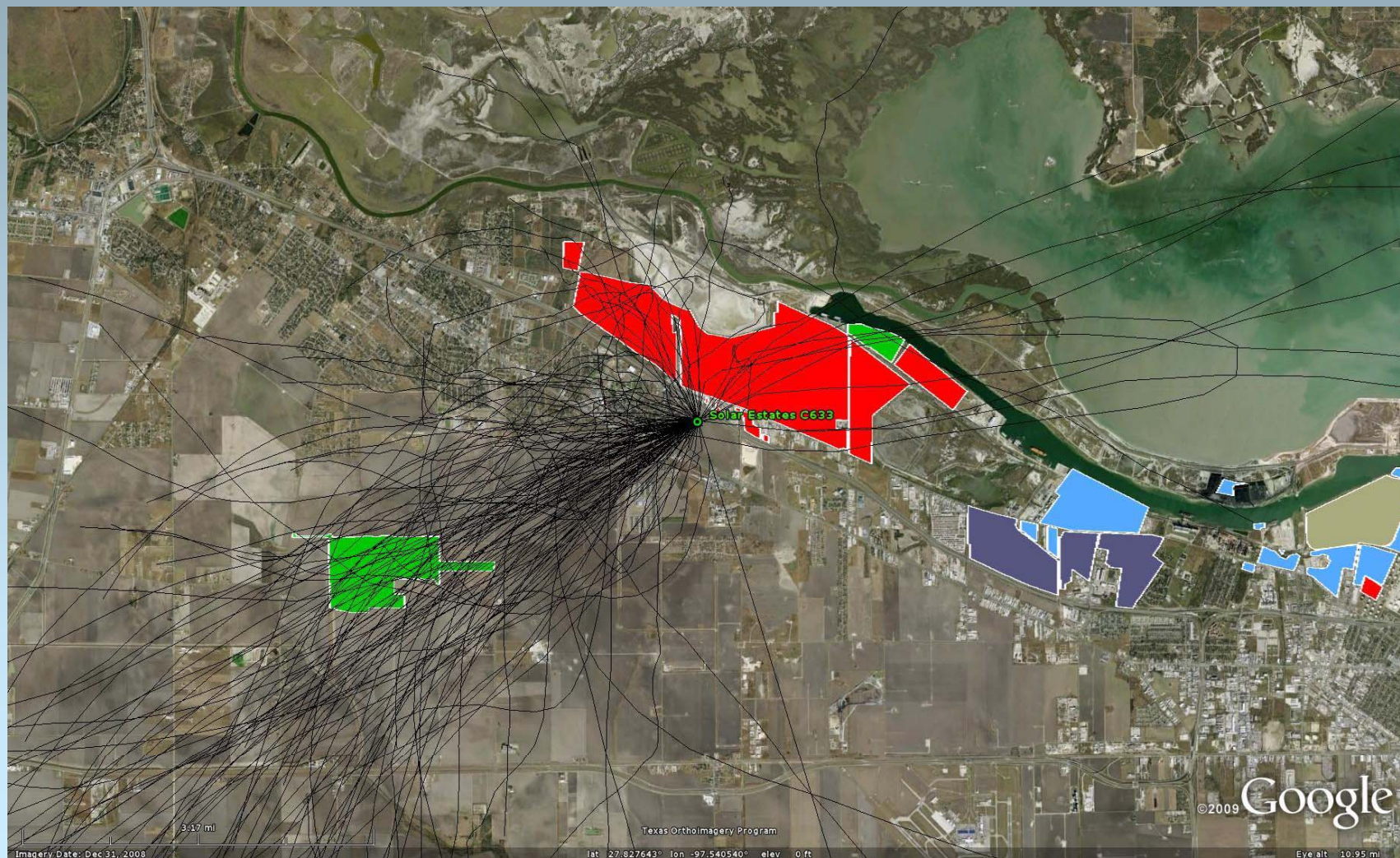
Oak Park



Solar Estates

- 1,3-butadiene concentrations at Solar Estates are higher than at Oak Park (note differences in scales).
- U.S. EPA's Toxics Release Inventories generally show an increase in 1,3-butadiene emissions between 2005-2008.

Upwind Source Regions when 1,3-Butadiene Concentrations are 5 ppbC or Greater at Solar Estates Based on Surface Wind Back Trajectories



Air Toxics Modeling Assessments in Corpus Christi

- Air quality modeling allows:
 - Concentrations to be estimated in areas without monitors.
 - Further understanding of air quality trends.
 - Indication of “hotspots” for future siting of monitors.
- Focus on benzene and 1,3-butadiene.
- Dispersion modeling using AERMOD and CALPUFF.
- Photochemical modeling using the Comprehensive Air Quality Model with extensions (CAMx) with meteorology from the Weather Research and Forecast Model (WRF).

Dispersion Modeling of Benzene Using AERMOD and CALPUFF: Emissions Inventory Assessment

- Initially focused on industrial point source emissions only.
- Investigated 13 inventories originating from the National Emissions Inventory (NEI), the Toxics Release Inventory (TRI) Program, the State of Texas Air Reporting System (STARS), and the photochemical modeling inventories used by the Texas Commission on Environmental Quality (TCEQ) to support State Implementation Plan development.
- Inventories have different origins, objectives, and spatial resolutions that can lead to pronounced differences in the inputs used for air quality modeling.

Emissions Inventory Assessment: TRI and NEI

- **Toxics Release Inventory (TRI)**
 - Origins in the Emergency Planning and Community Right to Know Act of 1986.
 - Annual reporting cycle for facility-wide emissions.
 - Does not provide emissions locations within property boundaries.
 - Examined 2002-2008 inventories for air emissions (stack and fugitive) in Nueces and San Patricio Counties.
- **National Emission Inventory (NEI)**
 - Three-year reporting cycle for criteria and hazardous air pollutants (CAPs and HAPs) to support mandates of 1990 CAAA.
 - Widely used for SIP development, compliance demonstrations, National Air Toxics Assessments (NATA), risk assessments.
 - Greater source resolution than TRI.
 - Texas submits data for both CAPs and HAPs. No reporting threshold for inclusion in the NEI submittal, i.e., all data reported through STARS database included.
 - Examined 2002 submittal and HAP NEI and 2005 HAP NEI submittal.

Emissions Inventory Assessment: TCEQ Photochemical Modeling Inventory

- Originates from the STARS database.
- TCEQ conducts additional processing to account for **rule effectiveness** and further **chemically speciate** emissions reported as VOC with unspecified composition.
- Rule effectiveness (RE)
 - Accounts for reductions in control efficiency.
 - Applied at the SCC/SIC/abatement level by geographic region.
 - Primarily affects VOC emissions from flares, equipment leak fugitives, external floating roof and internal floating roof tanks in Corpus Christi.
- Chemical speciation of VOC emissions
 - Needed to respond to regulations in the Houston area that target highly reactive VOCs.
 - *See Thomas et al. Emissions Modeling of Specific Highly Reactive Volatile Organic Compounds in the Houston-Galveston-Brazoria Ozone Nonattainment Area, presented at the 17th Annual International Emission Inventory Conference, Portland, OR June 2008).*
- Examined 2000 and 2005 inventories for San Patricio and Nueces County.

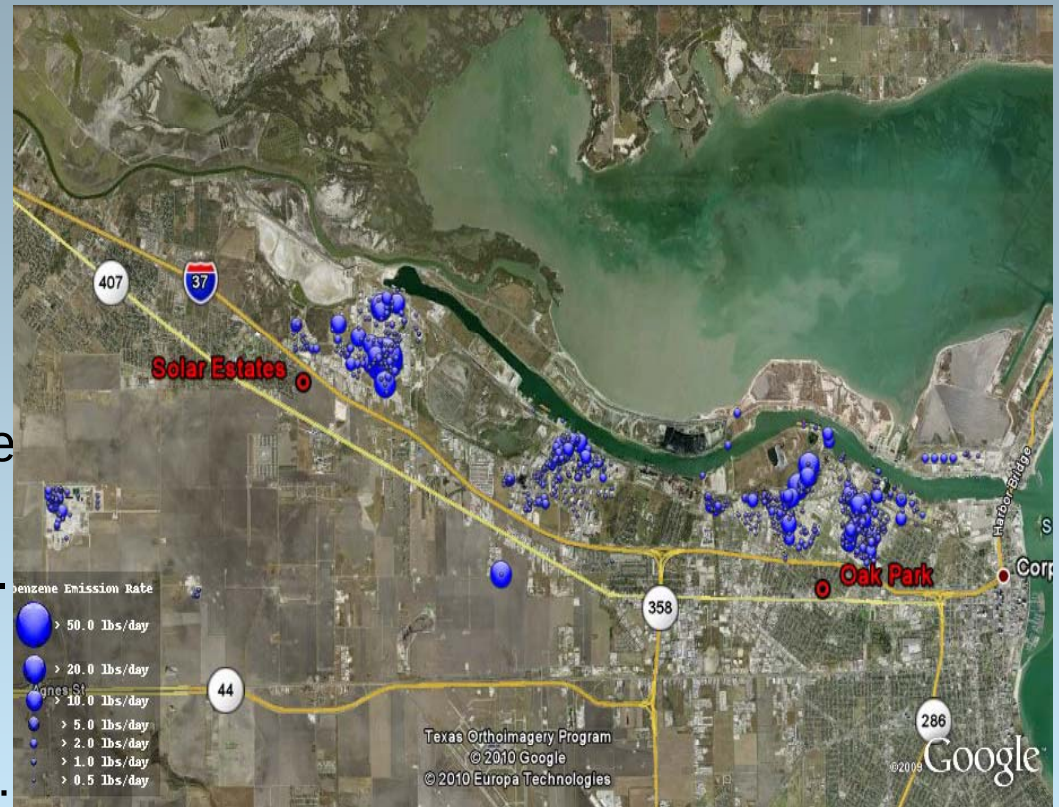
Comparison of Annual Emissions (tpy) of Benzene and 1,3-Butadiene in Nueces County

Species	2000 TCEQ Modeling EI	2002 HAP NEI	2005 TCEQ Modeling EI	2005 HAP NEI Submittal	TRI						
					2002	2003	2004	2005	2006	2007	2008
Benzene	248.2	166.8	259.3	93.5	109.0	123.8	120.4	104.9	84.4	78.7	76.5
1,3- Butadiene	0.0	0.99	7.0	4.9	1.4	2.9	5.4	5.6	13.5	6.7	9.4

Dispersion Modeling of Benzene Using CALPUFF

Point Source Emissions Inventory

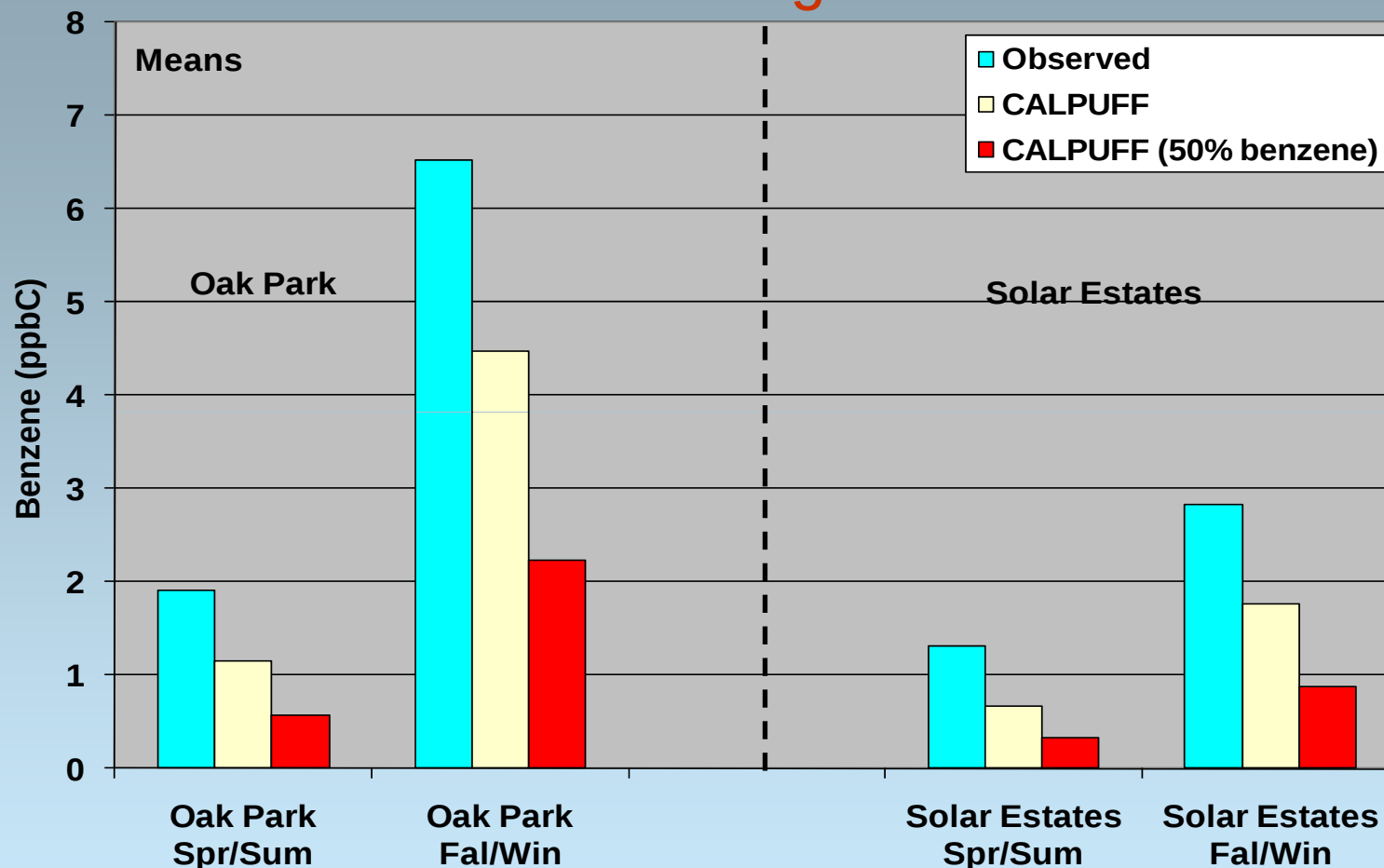
- Selected the 2005 TCEQ Photochemical Modeling Inventory, which included 1032 emission points. Tanks and fugitives were the most significant sources.
- Sensitivity study examined affects on model performance of 50% reduction in benzene emissions from point sources.



Meteorological Data

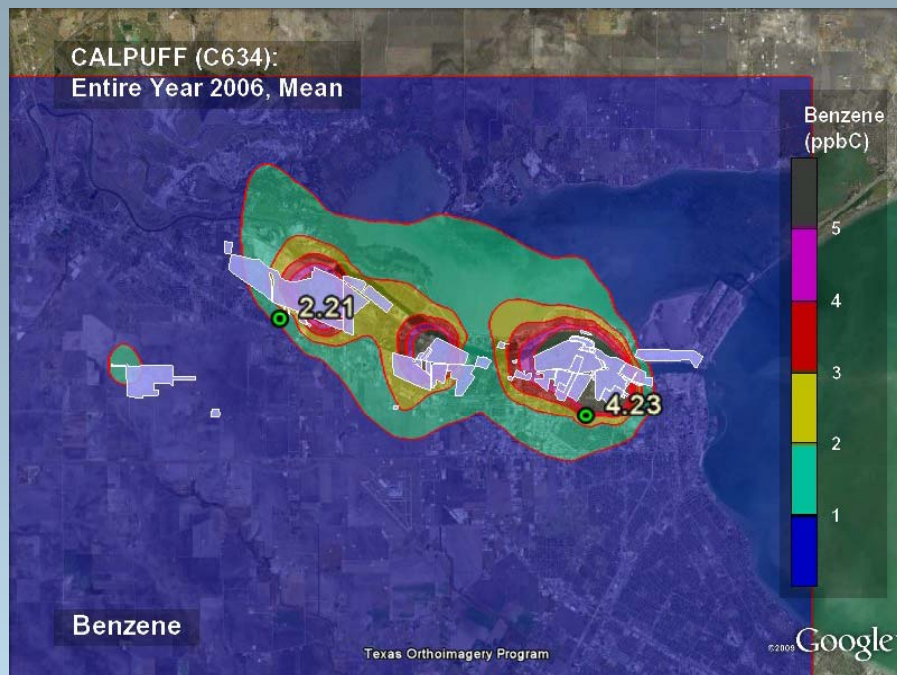
- CALMET: 18 surface stations; upper air data from the Corpus Christi International Airport; hourly buoy data for 2006-2008.

Observed and CALPUFF Predicted Benzene Concentrations at Oak Park and Solar Estates during 2006.

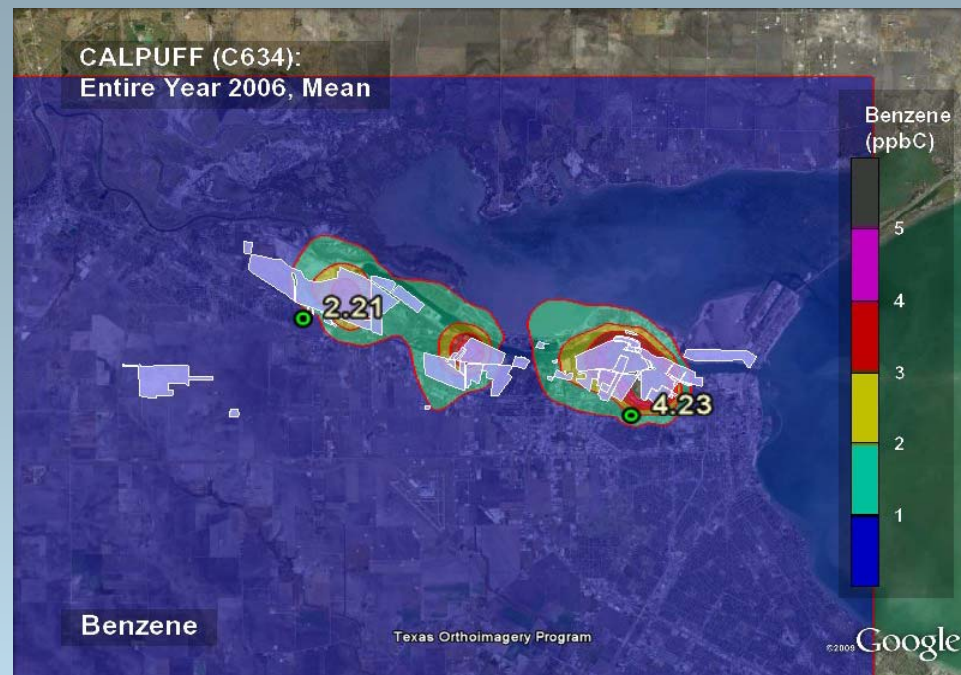


- CALPUFF replicates observed seasonal and locational differences.
- CALPUFF underpredicts observed concentrations; inventory comparisons suggest that chemical speciation of VOC emissions can be important for model performance.
- Estimated seasonal urban background contributions are approximately 1.2 ppbC during Fall/Winter and 0.6 ppbC during Spring/Summer at both sites.

Spatial Distributions of Mean Predicted Benzene Concentrations



TCEQ 2005 Photochemical Modeling EI



50% Reduction in the 2005 TCEQ
Photochemical Modeling EI

Note observed mean concentrations at the monitors and industrial point source property boundaries shown in gray.

- Spatial patterns are similar but smaller radius of influence with reduction in emissions.
- Current auto-GC sites are located within predicted radius of influence, but more central industrial area could be a focus of future monitoring.

Summary

- Emission inventories can have different origins, objectives, and spatial resolutions that can lead to pronounced differences in the inputs used for air quality modeling and evaluations of model performance.
- In this study, underlying differences between emissions inventories investigated for the Corpus Christi area were primarily related to the chemical speciation of emissions that were otherwise reported as VOC with unspecified composition and the accounting for rule effectiveness.