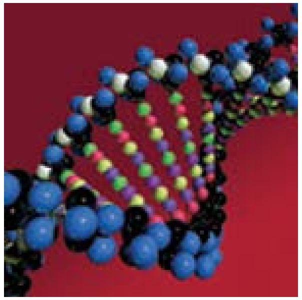
Transformation Rate of SO_2 to Sulfate for the Houston Ship Channel based on TexAQS 2006 Data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Background

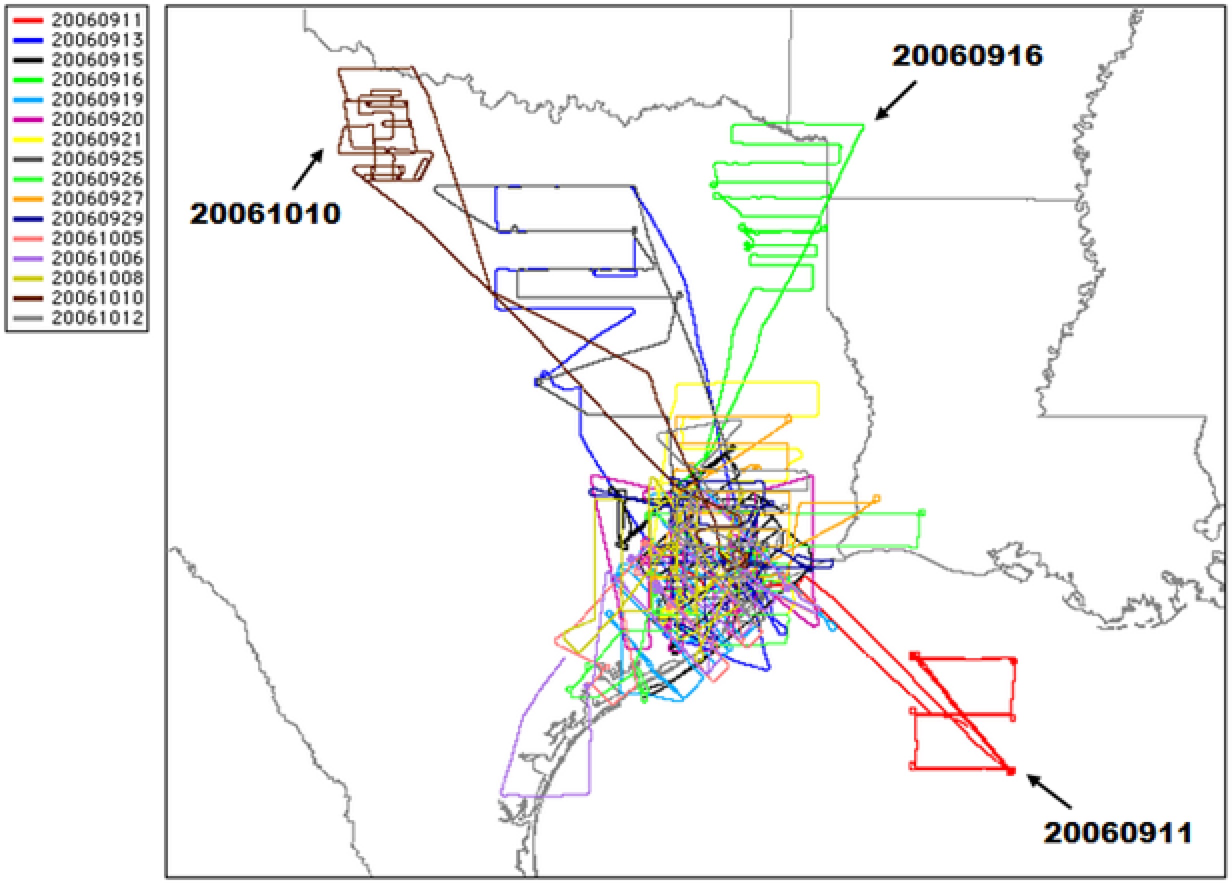
- In June 2010, U.S. EPA promulgated a new 1-hr SO_2 primary NAAQS
  - More stringent than previous: 75 ppb (1-hr SO_2) ← 140 ppb (24-hr SO_2)
    30 ppb (annual SO_2)
  - SIPs are due February 2014 that demonstrates compliance by August 2017
- AERMOD steady-state Gaussian plume model
  - EPA-recommended model for near-source 1-hr SO_2 modeling
  - Very simple treatment of chemistry (none or exponential decay)
- EPA guidance on 1-hr SO_2 NAAQS modeling
  - AERMOD regulatory default uses a half-life of 4 hours for modeling SO_2 in urban sources (zero conversion in rural)
  - May not be applicable for the Houston Ship Channel area

Development of SO_2 Conversion Rate

- Our goal is to develop SO_2 to sulfate conversion rate for HSC using the 2006 TexAQS data
  - High time-resolution data from the NOAA P-3 aircraft field campaign
- Direct analysis of conversion rate with the TexAQS data is difficult
  - Previous attempt showed that unique plume identification was difficult due to other local sources, complex meteorology, and background sulfate contributions
- We employed a modeling approach
  - Use the CAMx grid model with a simplified SO_2 conversion mechanism
  - Find the SO_2 to sulfate conversion rate that best fits the observation

NOAA P-3 Field Campaign during 2006 TexAQS

[Map from NOAA's 2006 TexAQS website]

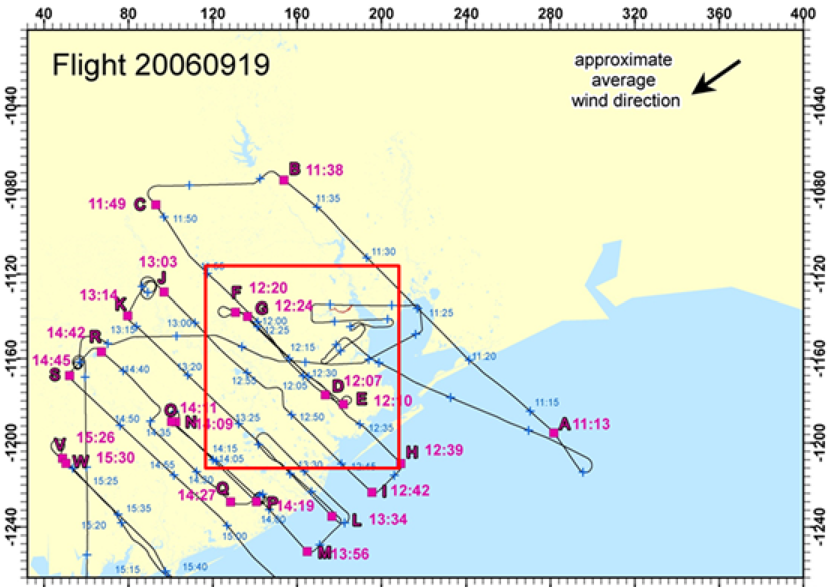


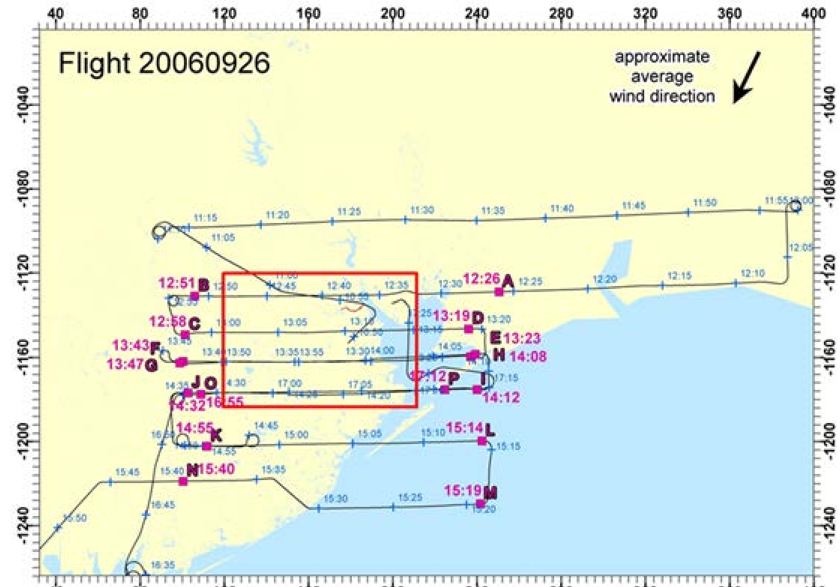
- Total 16 flights between September 11 and October 12, 2006
- 3 flights not focusing on HSC were prescreened

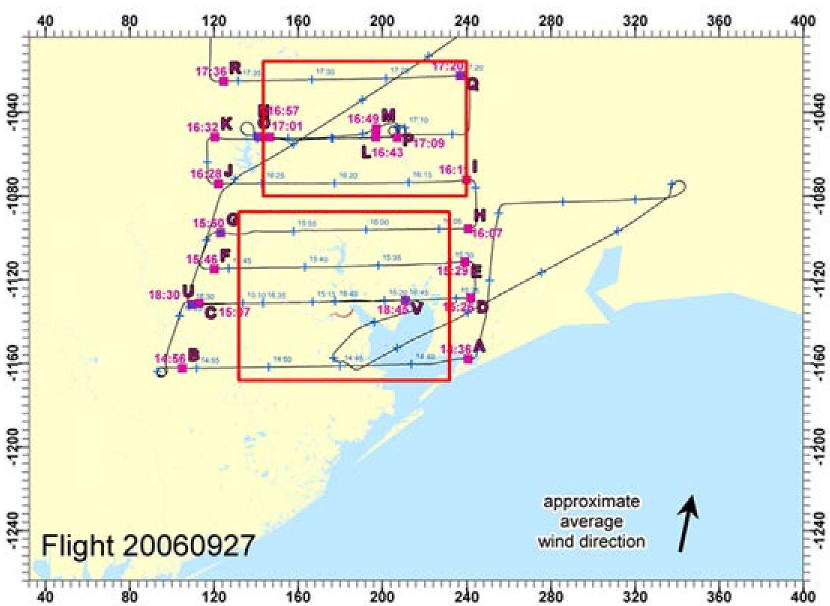
Flight Selection Criteria

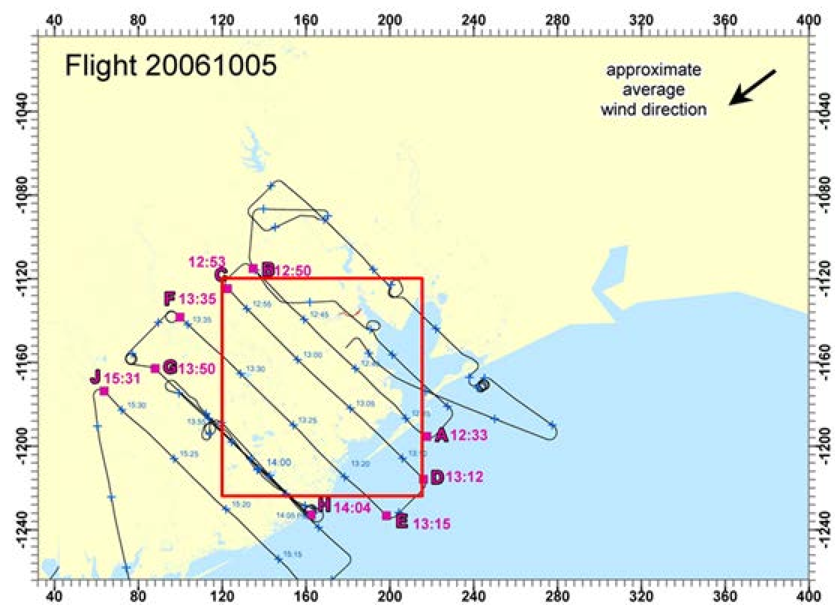
- Have more than one transect that show “complete” and “clearly distinguishable” Ship Channel plume
  - Drop ship channel plumes with missing data
  - Drop ship channel plume likely affected by local sources such as Parish power plant
- Have at least two transects with different distances from the Ship Channel sources
  - To verify reasonable SO_2 conversion by distance
- Ship channel plumes not too narrow to be modeled by the grid model
  - 1-km grid resolution for our modeling

Selected P-3 Flights









Grid Modeling

- Comprehensive Air-quality Model with Extensions (CAMx)
  - User-defined chemistry mechanism to mimic the first-order SO_2 decay in AERMOD:

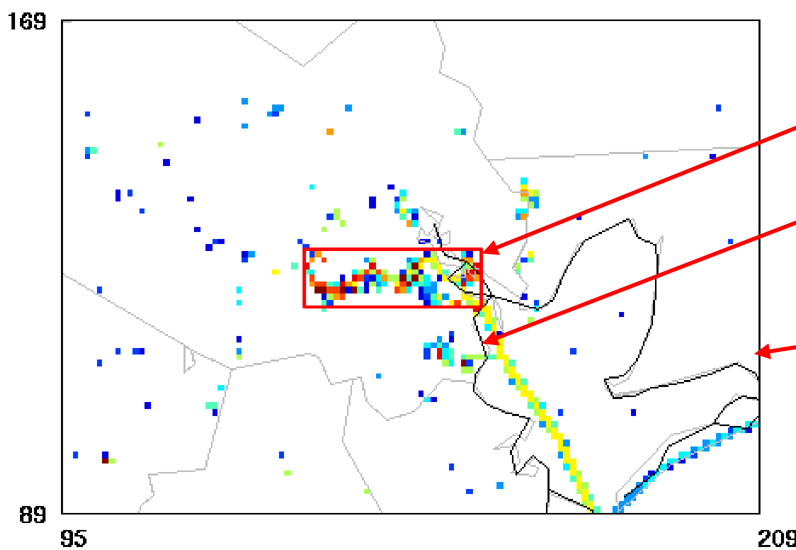
$$SO_2 \xrightarrow{k} SO_4$$

$$\frac{d[SO_2]}{dt} = -k[SO_2]$$

  - 4-km master grid centered on the HGB/BPA region with varying 1-km nested grids covering the HSC plumes
  - WRF modeling data and SO_2 emissions were provided by TCEQ
  - Boundary concentrations of SO_2 and sulfate for the modeling domain were extracted from previous CAMx modeling of North America

SO_2 Emissions

- TCEQ provided SO_2 emissions for the Houston region
  - Hourly emissions from major point sources (EPA’s Acid Rain database)
  - Other point source emissions from the ozone season database
  - Ship emissions
  - Area source emissions
- Model separately SO_2 (and sulfate) from:



Houston Ship Channel sources

All other sources within the modeling domain

Sources outside the modeling domain (through the BCs)

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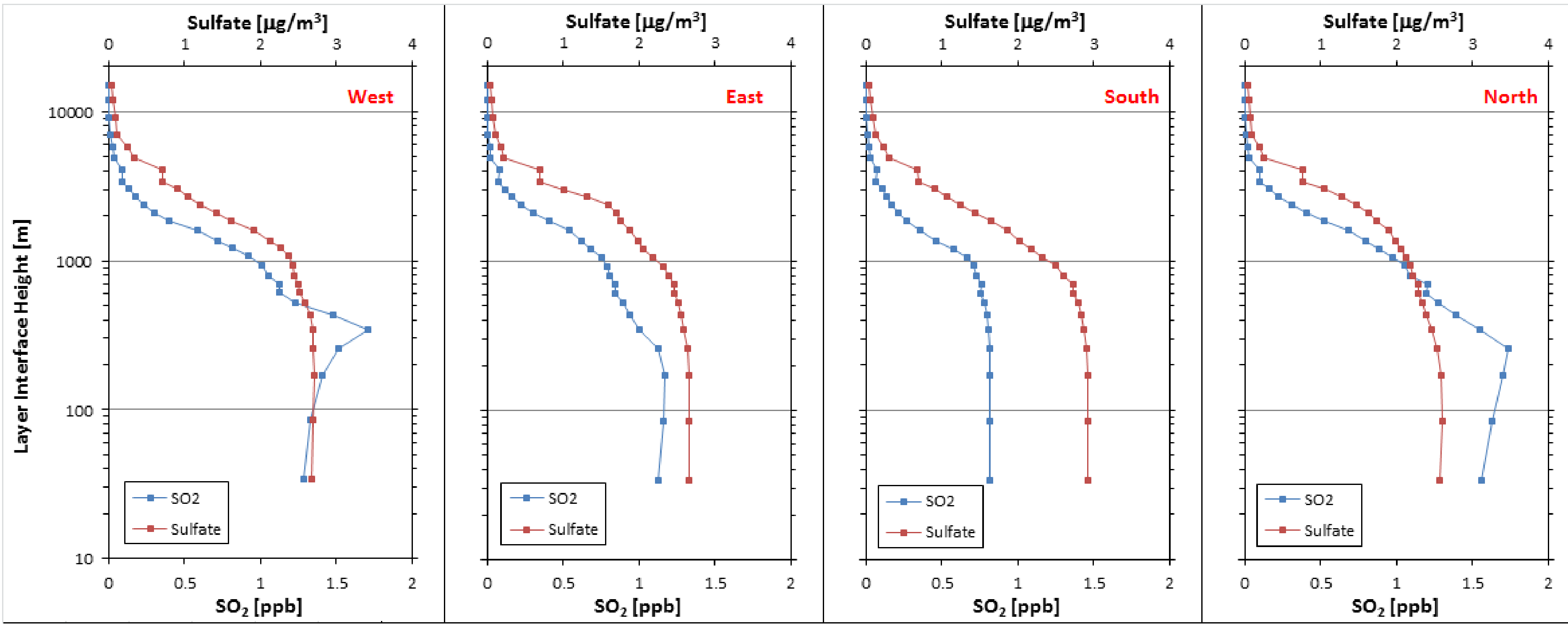
Boundary Conditions

- BCs extracted from the 2006 AQMEII NA modeling

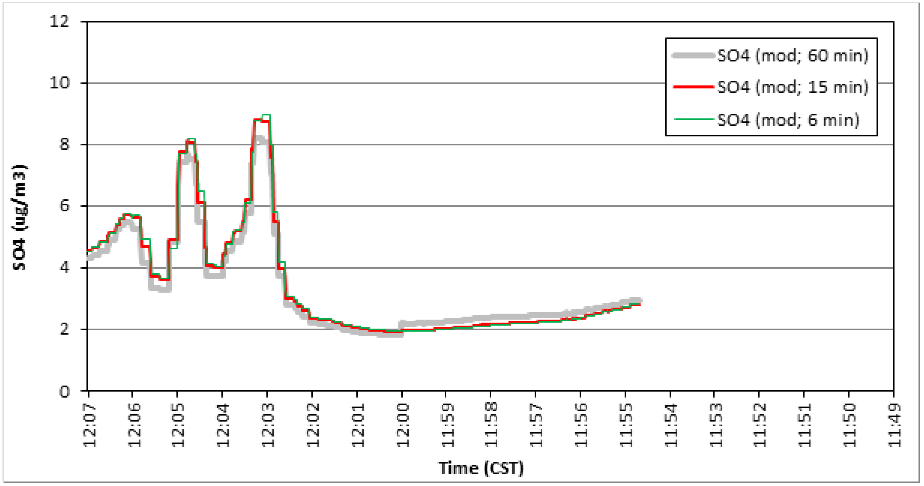


Episode-average vertical profiles of SO_2 and sulfate at each modeling domain boundary

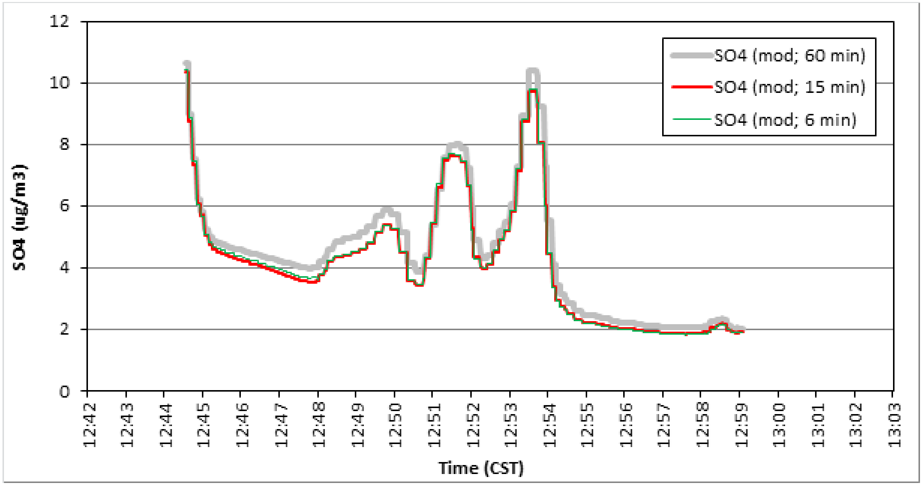
Model Output Frequency

- Different CAMx output intervals were tested
  - Hourly averages insufficient to capture fast progress of the plumes
  - 15-minute output interval seems adequate

Transect ~30 km from HSC



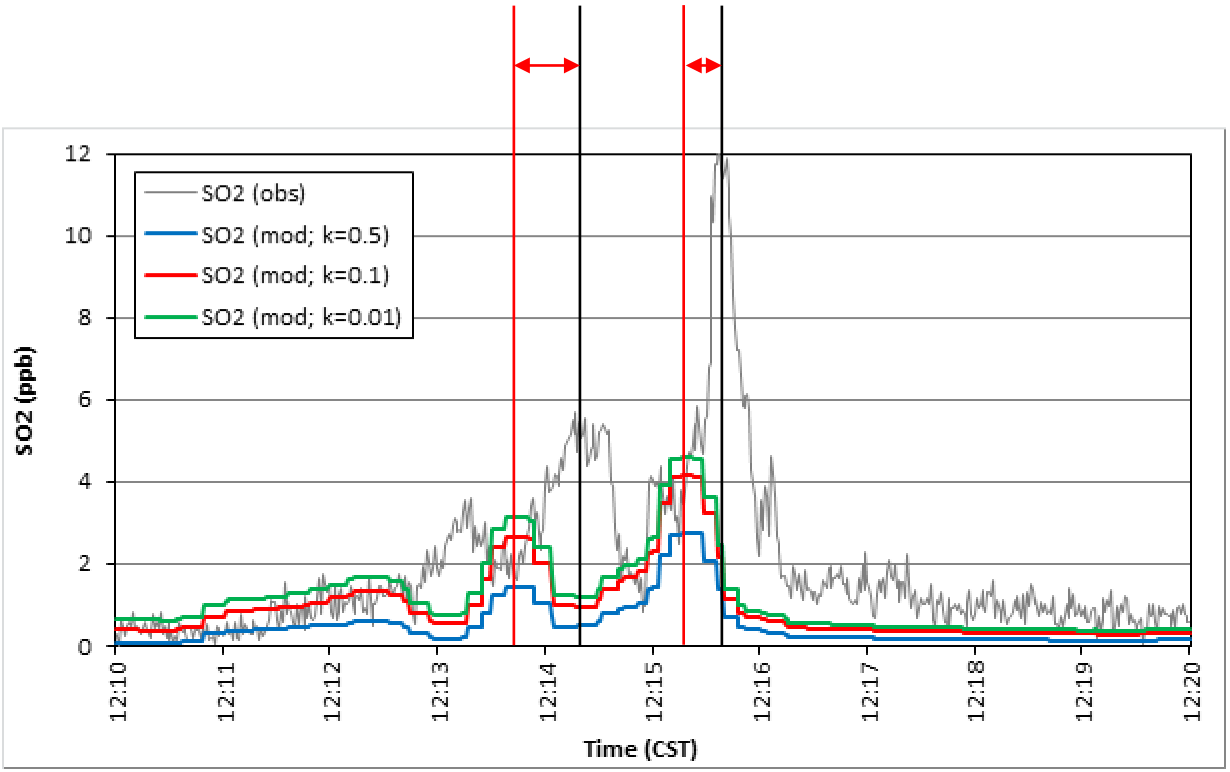
Transect ~50 km from HSC



Modeled SO_4 concentrations of the September 19 flight

Model Evaluation Issues

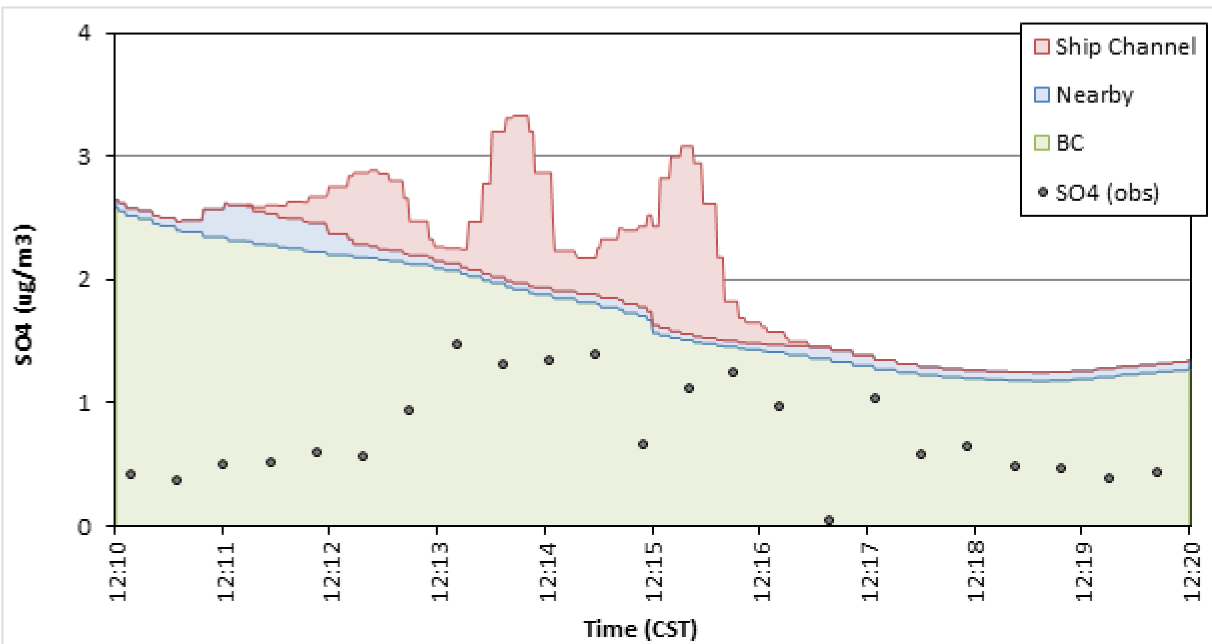
- Observed and modeled plumes are not exactly aligned due to inaccuracy in model met inputs



Observed and modeled SO_2 concentrations of the September 19 flight

Model Evaluation Issues

- Modeled background sulfate level appears too high



Observed and modeled SO_4 concentrations of the September 19 flight

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Model Evaluation Approach

- "Average excess above background" concentration is defined as follows:

$$\frac{\int (C - C_B)dt}{\int dt}$$

C : Total concentration
C_B : Background concentration

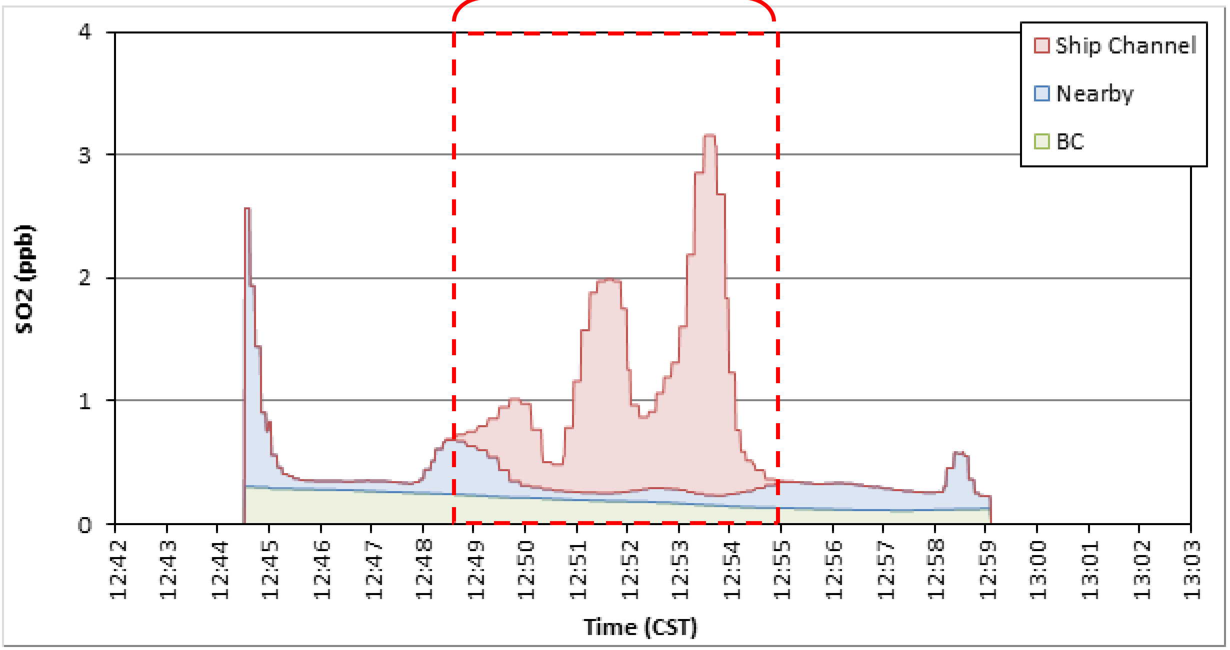
  - Normalized by plume width (represented by flight time, *t*)

Model Evaluation Approach

- The integration is limited to the transect segments representing the Ship Channel plumes

Ship Channel plume segment

Modeled



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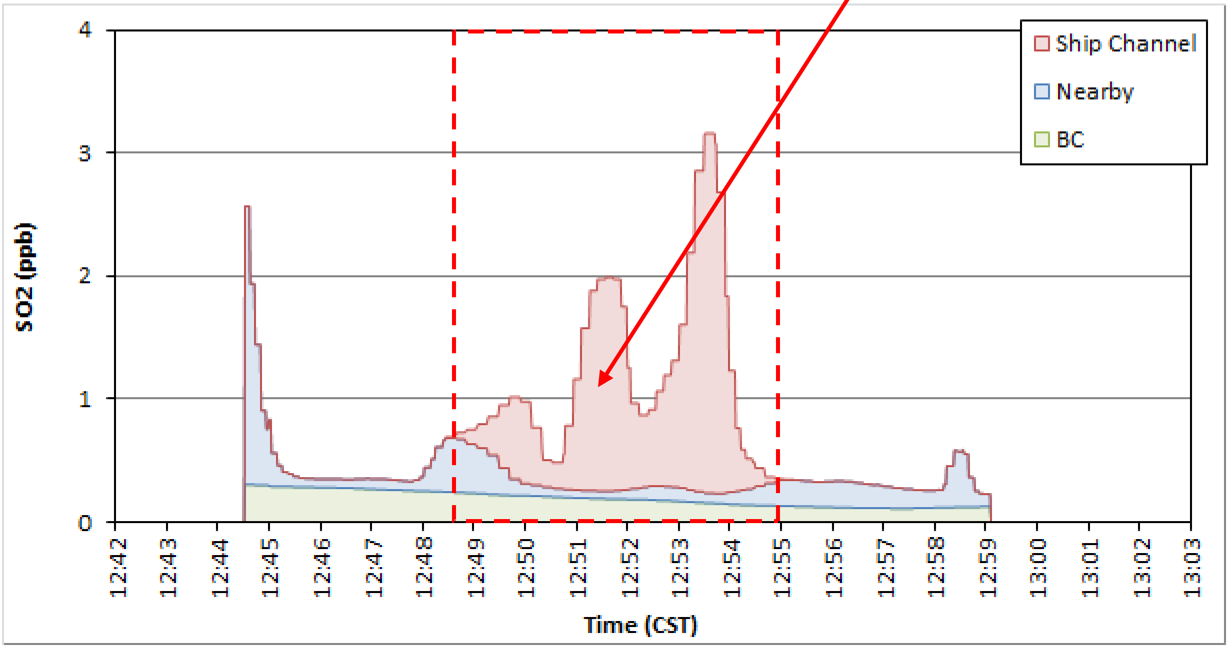
Model Evaluation Approach

- The integration is limited to the transect segments representing the Ship Channel plumes
- The Ship Channel contributions the model separately tracks represents the modeled “excess above background” concentrations

Modeled Ship Channel contribution

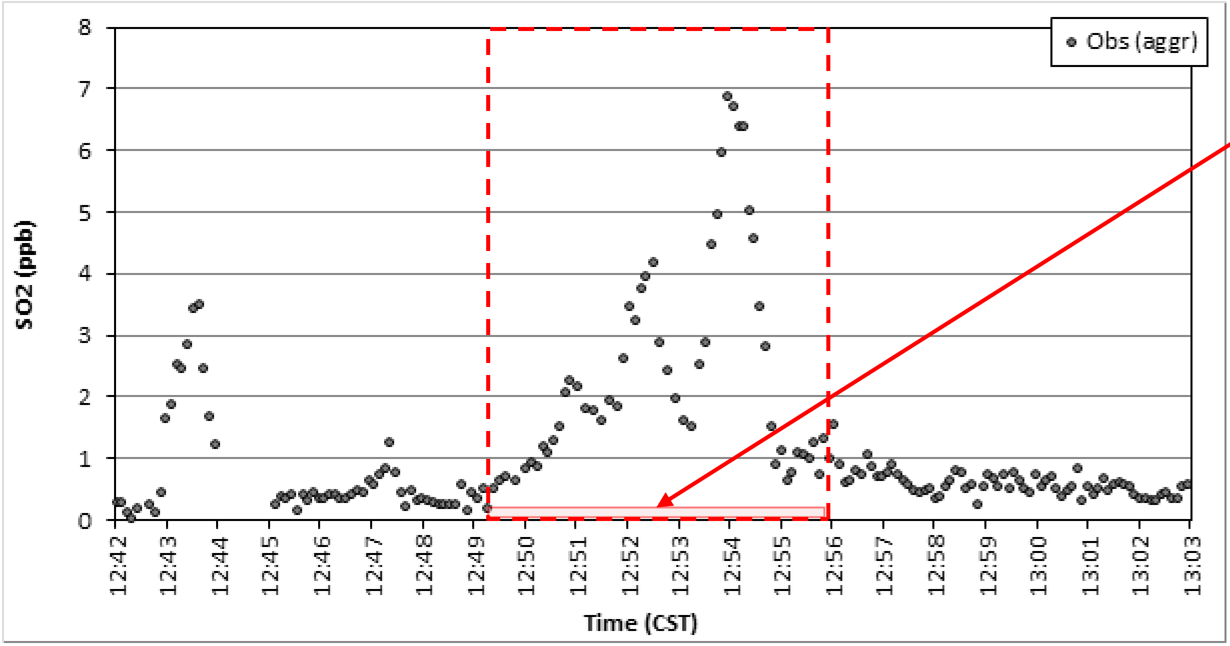
Modeled



Model Evaluation Approach

- The integration is limited to the transect segments representing the Ship Channel plumes
- The Ship Channel contributions the model separately tracks represents the modeled "excess above background" concentrations
- For the observed data, the background concentration is estimated as the minimum within the Ship Channel plume segment of the transect

Observed



Observed background concentration

Model Evaluation Approach

- Model evaluation was performed over the ratios of average excess SO_2 and sulfate concentrations

$$R_{\mathrm{AB}} = \frac{\text{average excess sulfate concentration for Transect A–B}}{\text{average excess } \mathrm{SO_2} \text{ concentration for Transect A–B}}$$

  - Transect segments that are missing measurement data for longer than 1 minute are excluded from the evaluation

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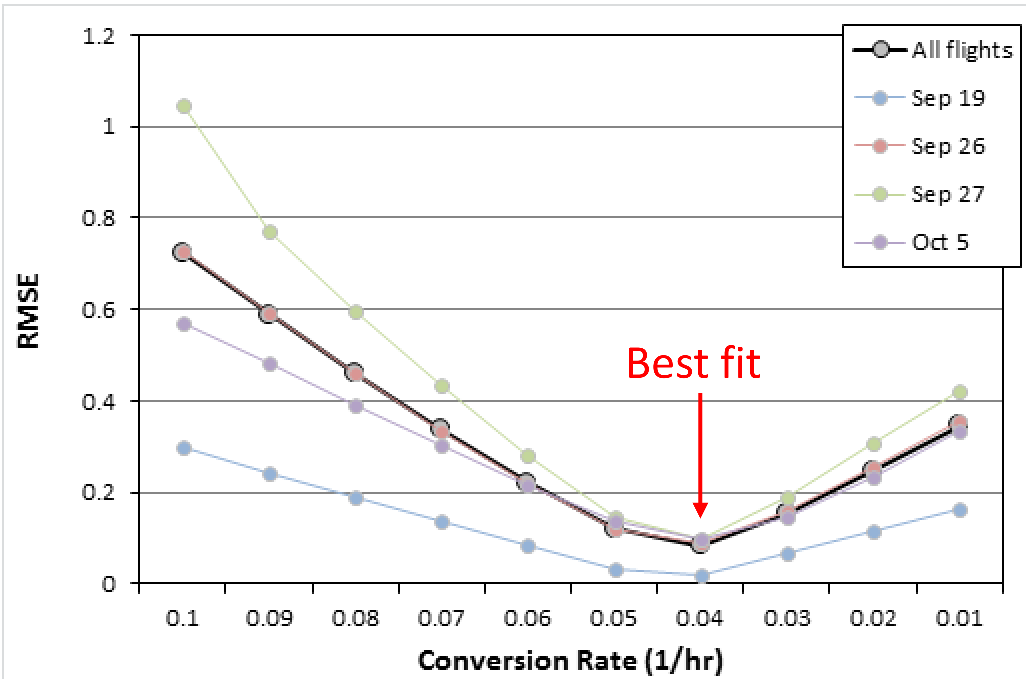
Model Evaluation Result



Root mean square errors of the average excess concentration ratio (*R*)

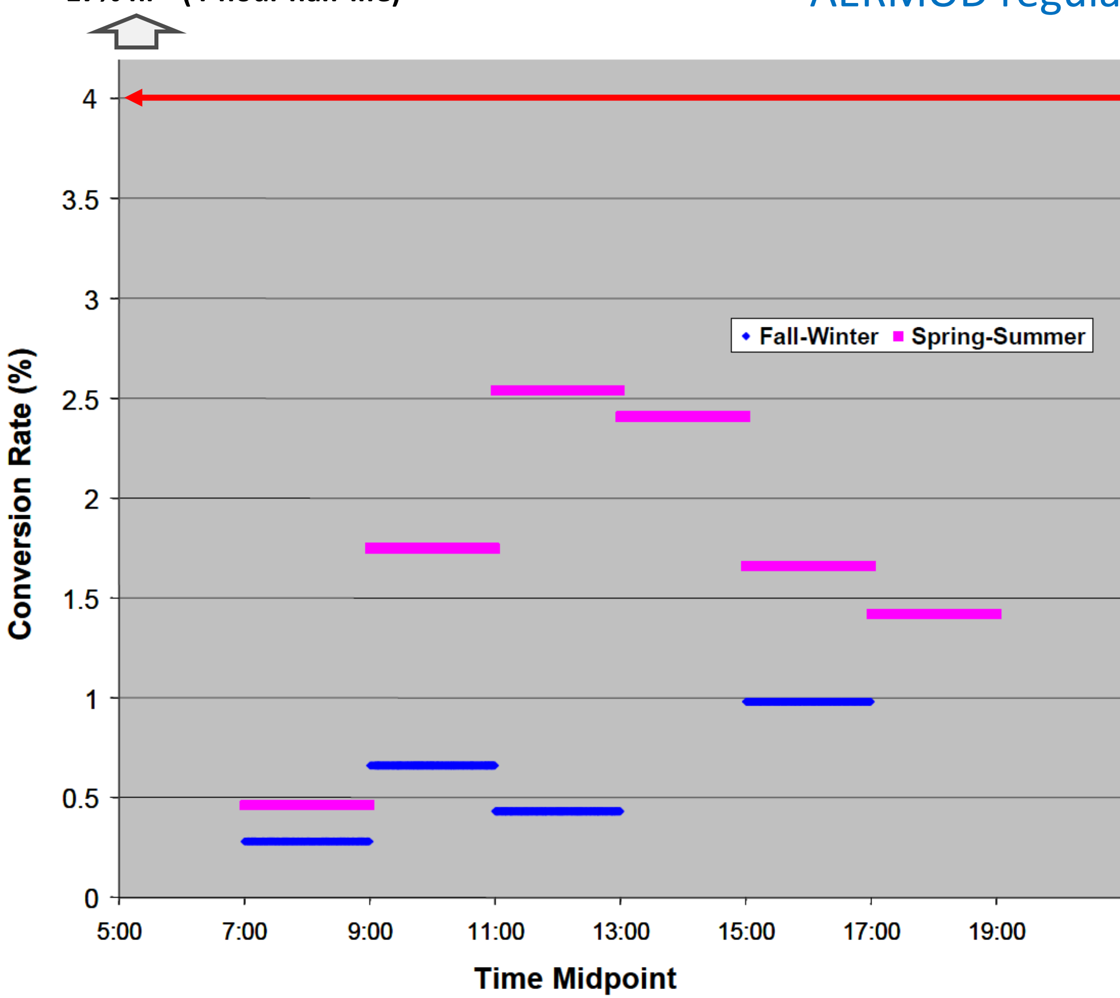
Comparison with Power Plant Plumes

- SO_2 conversion rate for HSC should be much higher than those for fossil-fueled power plants

> 17% hr^{-1} (4-hour half-life)

AERMOD regulatory default for urban sources

SO_2 conversion rate for HSC during TexAQS 2006



Mean SO_2 conversion rate for coal-fired power plant plumes estimated using SEARCH data

(Edgerton and Jansen, "An ARIES, SEARCH, and Mercury Update", ARA, May 2004)

AERMOD regulatory default for rural sources

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Summary

- The 2006 TexAQS field study data was used to develop SO_2 to sulfate conversion rate for the Houston Ship Channel that can be used with AERMOD to address the 1-hr SO_2 NAAQS.
- CAMx with AERMOD-style SO_2 conversion mechanism was applied to find the conversion rate that best fits the NOAA P-3 aircraft measurement data.
- Analysis using the “average excess above background” concentration ratio shows that a conversion rate of 0.04 hr^{-1} (half-life of 17 hours) best fits the observed plume data.
- Our result is based on flight data for ambient conditions of the Houston Ship Channel in late summer; caution is needed when applying to significantly different conditions (e.g., wintertime).

Acknowledgement

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