Potential Source Contribution Function (PSCF) Analysis of Highly Reactive Volatile Organic Compounds (HRVOC) Emissions in the Houston Ship Channel Area

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Overview

- Automatic Gas Chromatograph (Auto-GC) measurements of HRVOC concentrations in parts/billion (ppb) near the Houston Ship Channel over five years (2013 through 2017)
- Conditional Probability Function (CPF) for ethylene and propylene at Auto-GC sites
- Potential Source Contribution Function (PSCF) for ethylene using five-minute wind data at Auto-GC sites
- Composite PSCF for ethylene
- Composite PSCF for propylene
- Conclusions
Eight Auto-GC Sites in/around the Houston Ship Channel

Channelview
Wallisville
HRM 3
Lynchburg Ferry
Clinton Dr.
Milby Park
Cesar Chavez
Deer Park
Five Years of Ethylene and Propylene at Ship Channel Auto-GC Sites (90th Percentiles)

With a couple of exceptions, there appears to be little change in observed ethylene or propylene concentrations between 2013 and 2017. The 90th percentile values for the entire five-year window will be used in subsequent analyses. Note that observations with observed wind speed < 2 miles/hour are excluded.
Conditional Probability Function (CPF)

- Probability (empirical) that an air parcel arriving at a location from a specific wind direction contains a high concentration of a specified pollutant.

- For this analysis, the threshold value signifying a “high” concentration at a location is defined as the 90\textsuperscript{th} percentile of observed concentrations at that site over five years (2013-2017).
One-hour resultant wind direction was binned into 36 10° wedges. Each point represents the (empirical) probability that observed one-hour average ethylene at a receptor associated with a wind bin has a concentration greater than or equal to the 90th percentile of all ethylene concentrations observed at that receptor (minimum wind speed 2 mph).
CPF of Ethylene, 2013-2017

Circles represent a 60% probability that an observed ethylene concentration from a specific direction is ≥ 90th percentile of all observations.
CPF of Propylene, 2013-2017

Circles represent a 60% probability that an observed propylene concentration from a specific direction is ≥ 90th percentile of all observations.
Potential Source Contribution Function (PSCF)

• Similar in concept to CPF but uses trajectories to assign probabilities of high concentrations to locations rather than directions.

• Probability (empirical) that an air parcel passing through a grid cell arrives at a receptor carrying a high pollutant concentration.

• For example, count all back trajectories\(^1\) arriving at Deer Park that pass through a specific 1km X 1km grid cell \((i,j)\). Count those which carry pollutant above 90th percentile of all trajectories arriving at Deer Park.

• PSCF value for cell \((i,j)\) = \[
\frac{\text{# trajectories above 90}^{\text{th}} \text{ percentile at receptor}}{\text{Total # trajectories arriving at receptor}}
\]

\(^1\)For practical reasons, we actually count trajectory points, not the trajectories themselves.
Potential Source Contribution Function (cont.)

- Simple back trajectories constructed from 5-minute Continuous Ambient Monitoring Station (CAMS) data at each Auto-GC:
  - First convert 5-minute wind speed (WS) and direction (WD) to U-V components (in kilometers):

\[
U = - \frac{WS}{12} \sin(WD \cdot \frac{\pi}{180}) \times 1.60934 \\
V = - \frac{WS}{12} \cos(WD \cdot \frac{\pi}{180}) \times 1.60934
\]

- Work backward for desired number of time steps from Auto-GC location \((U_0, V_0)\):

Arrival at time \(t\)  
\(T-5\) min  
\(T-10\) min  
\(T-15\) min  
\(T-20\) min  
\(T-25\) min
• The trajectories used in this analysis only include data from a single site each. More sophisticated trajectory models can interpolate from multiple sites or use three-dimensional meteorological model output.

• To minimize wind speed and direction biases, trajectories were limited to no more than 36 points (three hours).

• To avoid measurement weirdness associated with low wind speeds, trajectories having scalar (path) length < 9 km were not used (3 km/hour is ~ 1.9 mph).

• Only trajectories arriving within the first 40 minutes of each hour were used, since the HGB auto-GCs typically sample air only during that time interval.
Potential Source Contribution Function (cont.)

- Count number of points in each 1 km X 1 km “cell”.

  - The map at right shows the base 10 log of the number of trajectory points surrounding the Deer Park site.

  - The maximum number of trajectory points for this map is 125,095 in the cell containing the site.
To ensure robust PSCF probability estimates, we only consider grid cells containing at least 500 points.

- The map at right shows the base 10 log of the number (≥ 500) of trajectory points in cells surrounding the Deer Park site.

- The maximum number of trajectory points for this map is 125,095 in the cell containing the site.
Of the grid cells shown on the previous slide, how many are associated with high ethylene at Deer Park?

- The map at right shows the base 10 log of the number of trajectory points in cells surrounding the Deer Park site that coincide with high (≥ 2.4 ppb) observed ethylene at the site (only cells with ≥ 500 total points).

- The maximum number of trajectory points for this map is 22,148 in a cell near the site.
The PSCF value in a cell is the number of high (≥ 90th percentile) concentration values divided by the total number of trajectory points in the cell.

- Air parcels passing through the orange-colored cells have a 60%+ chance of arriving at Deer Park with an ethylene concentration ≥ 2.4 ppb (the 90th percentile of all observed concentrations).

- Air parcels passing through the dark blue cells rarely, if ever, have ethylene concentrations ≥ 2.4 ppb.
Deer Park PSCF for Ethylene
(P90 = 2.4 ppb)
Channelview PSCF for ethylene
(P90 = 3.03 ppb)
Lynchburg Ferry PSCF for Ethylene
(P90 = 4.85 ppb)
HRM-3 PSCF for Ethylene
(P90 = 2.24 ppb)
Wallisville PSCF for ethylene
(P90 = 3.92 ppb)
Clinton Drive PSCF for Ethylene

(P90 = 2.81 ppb)
Milby Park PSCF for Ethylene
(P90 = 1.9 ppb)
Cesar Chavez PSCF for Ethylene
(P90 = 2.01 ppb)
Composite PSCF for Ethylene

- This map shows cells with one to eight monitors containing at least 500 trajectory points.
Composite PSCF for Ethylene

- This map shows the average PSCF value over all cells with at least one monitor having $\geq 500$ trajectory points.
Composite PSCF for Ethylene

- Average PSCF value over all cells with at least five monitors having \( \geq 500 \) trajectory points.

- Note color scale change.
Composite PSCF for Ethylene
This map shows the average PSCF value over all cells with at least one monitor having ≥ 500 trajectory points.
Composite PSCF for Propylene

- Average PSCF value over all cells with at least five monitors having $\geq 500$ trajectory points.

- Note color scale change.
Composite PSCF for Propylene
Conclusions

- PSCF can be a useful tool to locate areas associated with high concentrations of ethylene and propylene.

- Areas of high PSCF probabilities for ethylene and propylene are located very near each other.

- Use of a more sophisticated trajectory model could add support to the results presented here.
Questions?

The air modeling data analysis Section contributed to these results

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