

Appendix B.5

Phase 2 HGB Mid Course Review

Comparing the Emission Inventory to Ambient Data in Houston

J. Jolly, F. Mercado, and D. Sullivan

TCEQ

October 16, 2003

Appendix B.5

This appendix contains summaries of two data analysis projects that are closely linked, and which used the same methodology. The first report studies 12 different VOC classes, and the second report studies VOCs other than terminal olefins.

Comparing the Emission Inventory to Ambient Data in Houston

J. Jolly, F. Mercado, and D. Sullivan

October 16, 2003

Background:

It has become well understood in the last few years that highly reactive VOCs are underreported, sometimes greatly, in the Houston emission inventory. Work done in 2002 by TCEQ staff¹ compared reported point source emissions of several highly-reactive VOCs in the Houston area with ambient data collected by five Auto-GCs in the area. This study estimated that these emissions were underreported by as much as 96 times, depending on the VOC and the source cluster involved. But this study did not address non-point sources of emissions, nor did it look at VOCs other than the few that were studied.

Project Description:

This project was intended to expand upon the work done in the earlier study. It follows the same basic methodology: each monitor's ambient data was subdivided, according to wind direction, into 36 ten-degree wind bins, and VOC:NOx ratios of emissions sources within each bin were compared (after converting from mass to volume units) with the same ratios from the ambient data falling into that bin. The median of all ambient ratios, for each bin, was used for comparison.

There were several methodological differences between this study and the earlier one, however. This project included emissions from area, mobile, nonroad, and ship sources, in addition to point sources. Emissions were weighted by the inverse of the distance from the source to the monitor. Long-term data from two area monitors (Clinton CAMS 403 and Deer Park CAMS 35) were used, rather than five monitors. Only sources located within 14 km of one or more of the monitors were included. Finally, 12 different VOC classes were compared, rather than just ethylene and propylene.

¹ Estes M., J. Smith, J. Price, G. Cantu, D. Boyer, Z. Fang, and J. Neece (2002). *Preliminary Emission Adjustment Factors Using Automated Gas Chromatography Data*. Attachment 7, Technical Support Document of the TCEQ Executive Director Recommendation for Changes to Chapter 115/117/101 Rules, November 11, 2002. ftp://ftp.tnrc.state.tx.us/pub/OEPAA/TAD/Modeling/HGAQSE/Modeling/Doc/TSD_PHASE1/attachment7-agc_ei_adjustment.pdf

Maps of point source emissions in the area revealed that they were often clustered in groups that span two or more wind bins. For directions dominated by point sources, emission ratios for an entire cluster – spanning from one to eleven wind bins – were compared with ratios from ambient data spanning the appropriate bins.

Results:

It was found that directions dominated by non-point sources had generally better agreement between emissions and ambient ratios than did those dominated by point sources, suggesting that the non-point inventory is more accurate. Results for less-reactive VOCs were not appreciably different from those of highly-reactive VOCs. The butanes class (consisting of isobutane and n-butane) was unique among the twelve classes studied, in that its emission ratios were often considerably less than ambient ratios in both point and non-point dominated source regions.

For the point source clusters described above, emission adjustment factors were developed; these were simply the ratio of ambient to emissions VOC:NOx ratios for the bins covering a cluster. For most clusters, and most VOC groups, adjustment factors ranged from 1 to 6, meaning that emissions would have to be multiplied by a factor somewhere in that range to achieve unity with the ambient data. Notably at Clinton, butenes (1-butene, c-2-butene, t-2-butene) from wind directions 130-200 were found to be underreported by a factor of ten. At Deer Park, four classes had adjustment factors exceeding 6:

- butanes from 120-140 compass degrees (adj. Factor = 10);
- C5_cyclos from 350-10 degrees (factor = 13.6);
- C6_cyclos from 20-60 degrees (factor = 12.1);
- Ethylene from 350-10 degrees (factor = 11.9).

Development of Adjustment Factors for VOCs other than Terminal Olefins

J. Jolly, F. Mercado

March 11, 2004

A comparison of ambient to emissions VOC:NOx ratios was conducted by TCEQ staff in October, 2003. In this comparison, ambient data from two auto-GC monitors in the Houston area for the years 1999 through 2001 were compared to the emission inventory during that time. Ambient data from Deer Park and Clinton, the two monitors used in the study, were subdivided into 36 bins based on resultant wind direction, with each bin comprising ten degrees. Mean ambient ratios were calculated for each of these bins for each of the two monitors, and for each of 12 different VOC classes.

To calculate the corresponding emission VOC:NOx ratios, a polar grid consisting of 36 equally-sized cells, shaped like pie slices, was created for each monitor, with the monitor located at the center of the grid. Each of the two grids was 28 km in diameter; each grid cell had a radius of 14 km and was ten degrees wide, corresponding to the same ten degrees forming each wind bin. Within each grid cell, VOC:NOx ratios for each of the 12 VOC classes were calculated using emissions from all anthropogenic sources in the cell, including point, area, nonroad, mobile, and ship sources. All emissions were weighted by the inverse distance from the source to the monitor before calculating the cell's VOC:NOx ratios.

If it is assumed that the monitor data are accurate, and an accurate emissions inventory would have VOC:NOx ratios equal to those measured at a nearby monitor, then the ratio of ambient to emissions VOC:NOx ratios can be considered to be an "adjustment" factor that can be applied to the emission inventory, in order to make it correct. These factors were calculated for each of the VOC classes and for each bin at both monitors.

For bins dominated by point source emissions, adjustment factors were calculated for "wedges" of one or more contiguous bins. These wedges corresponded to the location of point source clusters within each grid. The wedges defined at a monitor sometimes varied by VOC class. For each wedge, adjustment factors were created. Depending on the size of the point source cluster and its distance from the monitor, a wedge could span anywhere from one to eleven bins in size. This process resulted in 15 wedges around Clinton, and 27 around Deer Park.

The adjustment factors calculated for each of these 42 wedges were used to calculate an adjustment factor for VOCs other than terminal olefins. This was done as follows: for each monitor, adjustment factors for those wedges containing entirely or partly terminal olefins were excluded from calculation. This resulted in the exclusion of the following VOC classes: butadiene, ethene, propene, butenes, and pentenes. For the remaining 22 wedges (eight at Clinton, and 14 at Deer Park), average adjustment factors were calculated for each monitor. The average of the two monitors' averages was 4.5 – this represented the final adjustment factor. An earlier analysis had excluded only butadiene, ethene and propene from calculations. The adjustment factor resulting from that earlier

analysis was 4.8, and was the factor used in sensitivity modeling, conducted in support of the 2004 SIP revision, to consider the effects of adjusting the base- and future-case other reactive VOC emissions.