Ground Truth Verification of Emissions in the Houston Ship Channel Area
Revised Final Report

STI-900650-2161-RFR

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August 30, 2002
This final report was prepared for the Texas Natural Resource Conservation Commission Modeling Assistance Project II, Work Order Number 31985-15.
1. INTRODUCTION

The purpose of this work order was to work cooperatively with industry to (1) assess point and area source emissions and activity data for industrial facilities in the Houston Ship Channel (HSC) area; (2) provide an independent, overall quality control and quality assurance check of emission estimation procedures (e.g., track emissions as reported by individual facilities to emissions for the same facility as stored in the TNRCC database for use as input to air quality models); and (3) provide recommendations for steps to improve emission estimation and/or reporting procedures. These tasks encompassed the assessment of emissions in a highly complex industrial setting. To the extent possible, differences between annual emissions and actual day-specific, hourly, or batch operations as well as fugitive, stack, or process emissions were also examined.

This report summarizes the work conducted and the findings based on site visits to eight facilities that represent an array of reactive volatile organic compound (VOC) emission sources for petrochemical facilities of varying sizes near the HSC. Specific findings from individual facilities are not detailed in this report. Instead, statistical summaries of findings from all facilities combined were prepared.

As stated in the original scope of work, “[t]he success of this type of study is directly related to the cooperation of industry sources (e.g., providing on-site access and access to site-specific air emissions permit staff for consultation).” Sonoma Technology, Inc. (STI) is pleased to report that each of the facilities visited during this phase of the study worked in an extremely open and cooperative fashion. Access to key personnel and equipment at each facility was exceptional.

This report includes (a) a description of the on-site ground truth activities conducted during winter 2001-2002, (b) statistical summaries of emission discrepancies (based on individual facility results), and (c) recommendations to improve emission estimation and/or reporting procedures.

2. TECHNICAL APPROACH

STI acquired emission estimates and the number of point emission sources for petrochemical facilities in the HSC from the TNRCC. Facilities were sorted and ranked by their emissions of VOCs and nitrogen oxides (NOx) and number of emissions point sources. From this list, a subset of facilities (small, medium, and large) was randomly identified. Working in cooperation with the TNRCC, STI held a meeting in the HSC area in December 2001 to recruit volunteers from this subset of facilities to participate in the on-site ground truth efforts. Ten facilities agreed to participate; however, due to logistical coordination issues during the time allowed to complete the ground truth surveys, site visits could only be carried out at eight facilities. STI and TNRCC representatives completed visits to seven facilities near the HSC—Goodyear, Exxon-Mobil, Texas PetroChemical, Aristech-Sunoco, Rohm & Haas, BP Solvay, and Shell Chemical; and one facility at Sweeny, Texas—Chevron-Phillips.
Site visits were designed to be completed in two days:

Day 1: STI and TNRCC representatives met with site personnel to complete introductions, review site safety procedures, allow site safety engineers to approve STI’s on-site use of a global positioning system (GPS) and palmtop computer, and obtain approval for site access. Each facility provided a lecture-style overview of the processes and production lines present at the site. STI and TNRCC were then escorted on a tour of each facility. Near the end of the first day, STI provided facility operations personnel with a copy of data from the TNRCC’s emission inventory records for their facility for review on Day 2.

Day 2: STI and TNRCC conducted a review of TNRCC’s emission inventory data with facility operations personnel. Detailed discussions with site personnel about the inventory data were undertaken, and the site was toured again as necessary to examine individual emissions points. Any discrepancies were identified and resolved (if possible). Unresolved issues were summarized for follow-up by site personnel, STI, and/or TNRCC.

To prepare for the site visits, STI reviewed the emission inventory data for each facility. STI spot-checked data records from TNRCC’s emission inventory files against the records that were made available by operations staff for each facility. While on-site, we systematically checked the largest five or six sources of emissions and spot-checked several smaller sources. During site visits, we also reviewed the general procedures that facilities used to estimate and report their emissions.

STI mapped the locations of EPNs using ARCView and overlaying the results on aerial photographs of the study area. Maps of emissions points for each facility were provided to each facility during the site visits. During the site visits, STI investigated the locations of emissions points that had off-property coordinates and were likely to be errant. Emission point numbers (EPN) for the likely errant points were highlighted and brought to the attention of operations personnel at each facility. At the sites, STI also performed random spot checks of coordinates for emissions points that were located within plant property lines. The results of the investigations of location-related information are summarized in Table 1 in Section 2.1, Key Findings, of this report.

The emission assessments conducted in this study also included limited comparisons of point and fugitive emission source characteristics (e.g., stack parameters, such as stack heights, diameters, flow rates, and temperatures) and emissions estimates with readily available data for similar petrochemical sources in other areas of the United States. The results of these comparisons are provided in Section 2.1 of this report.

Information about emission estimation methods and reporting methods used by each facility was obtained through interviews with operations staff at each facility during on-site visits, coupled with follow-up telephone calls.
2.1 **KEY FINDINGS**

### 2.1.1 Reconciliation of Point Source Emissions Locations

Table 1 summarizes the results of the reconciliation of point source emission locations. TNRCC records show investigation of a combined total of 1823 EPNs at the eight facilities participating in the study. STI reconciled location information by mapping the EPNs using ARCView (and translating coordinates to the 1983 North American Datum\(^1\)) and overlaying the results on aerial photographs of the study area. By number count, nearly all of the EPNs were correctly positioned within property boundaries. The small number of EPNs located beyond the property boundaries included retired or inactive sources with no emissions as well as active sources with emissions. Although the number of mislocated EPNs or EPNs with missing coordinates is quite small, the emissions associated with them could be important. The emissions associated with location problems for active EPNs ranged from an insignificant fraction to about 10 to 15\% of an individual facility’s total VOC or NO\(_x\) emissions. No significant errors were identified during spot checks of point source locations within the fence line during site visits.

#### Table 1. Summary of reconciliation of point source emissions locations.

<table>
<thead>
<tr>
<th>Type of Emissions Points</th>
<th>No. of Points</th>
<th>% of Total</th>
<th>VOC (TPY)</th>
<th>% of Total</th>
<th>NO(_x) (TPY)</th>
<th>% of Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total EPNs:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total for 8 facilities</td>
<td>1823</td>
<td>100%</td>
<td>4,720</td>
<td>100%</td>
<td>9,404</td>
<td>100%</td>
</tr>
<tr>
<td>Mislocated active EPNs:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total for 8 facilities</td>
<td>38</td>
<td>2.1%</td>
<td>19.0</td>
<td>0.4%</td>
<td>415</td>
<td>4.4%</td>
</tr>
<tr>
<td>Outside property line:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>At any distance</td>
<td>18</td>
<td>1.0%</td>
<td>10.0</td>
<td>0.2%</td>
<td>146</td>
<td>1.6%</td>
</tr>
<tr>
<td>More than (\frac{1}{2}) km</td>
<td>7</td>
<td>0.4%</td>
<td>1.6</td>
<td>0.03%</td>
<td>146</td>
<td>1.6%</td>
</tr>
<tr>
<td>Missing coordinates</td>
<td>20</td>
<td>1.1%</td>
<td>9.0</td>
<td>0.2%</td>
<td>268</td>
<td>2.8%</td>
</tr>
</tbody>
</table>

\(^1\) During the process of creating the facility maps, STI inferred that TNRCC emission inventory data are projected using the 1927 North American Datum (NAD27). Most satellite-derived data, such as satellite photographs of the earth’s surface, are currently projected using the 1983 North American Datum (NAD83). When multiple databases (e.g., land-use maps, aerial photographs, etc.) are brought together in a geographic information system (GIS), a common single datum is preferable. The use of a consistent projection datum is particularly important when combining various inputs (including emissions, land use, and meteorology) for use in air quality models. Although the error between NAD27 and NAD83 is relatively small—about 200 hundred meters or so in the HSC area—it can be important for certain applications, such as reconciling individual point source emissions locations or selecting sites for air quality monitors.
2.1.2 Assessment of Point Source Characteristics

Emissions and source characteristics were obtained from TNRCC for each of the largest VOC and NOx sources at each facility examined in the ground truth study. The resulting 16 EPNs investigated included 4 flares, 3 fugitive sources, and 9 stacks; the single largest EPNs had individual emission rates of nearly 350 tons of NOx per year and about 200 tons of VOCs per year. For stack sources, specific parameters examined included stack height and diameter, exit temperature, and exit velocity. For flares, flow rate, heat value, and molecular weight were examined in addition to stack characteristics. Fugitive emissions parameters examined included the reported length, width, height, and directional orientation of the fugitive source area.

No significant discrepancies were found in the source characterizations made in this evaluation. In general, the parameters reported by the examined facilities were consistent with sources of similar size and type at other petrochemical facilities in the western United States.

2.1.3 Emission Estimation Methods

A variety of emission estimation methods are employed at the eight facilities investigated, ranging in use of published U.S. Environmental Protection Agency (EPA) software (e.g. TANKS) to custom-built in-house electronic spreadsheets and third-party software. Examination of the tools used by the facilities show that procedures to estimate routine emissions followed EPA- or TNRCC-recommended estimation methods.

2.1.4 Emission Reporting Methods

A variety of reporting methods are employed at the eight facilities investigated, ranging from handwritten entries on paper copies of TNRCC-supplied emission reporting forms to electronic submission using third-party software. Of the eight facilities visited, four (or five—one site was not sure of the electronic reporting software’s name) use a commercially available software package called “WINCEIS”, and the remaining three manually report emissions using paper forms.

Three facilities had potentially significant reporting errors identified during the ground truth exercise. The first facility had a discrepancy between the speciated sum total and the reported total of VOC emissions in the TNRCC emissions database. This facility reported total VOC emissions of about 500 tons per year. However, when the sum of reported speciated VOC emissions was calculated, the sum is about 830 tons per year. While at the facility, a misinterpretation of handwriting was noted during spot checks of the inventory. For example, a handwritten "4" looked like "9", so that for one source, a 50-ton difference was found, when “40” was misinterpreted as “90”. We did not verify all records to fully reconcile the remaining 330 ton discrepancy. There was also a discrepancy between the reported total and VOC and sum of speciated VOC emissions at a second facility. The difference between the sum of speciated VOCs and reported total VOCs for this facility was about 10% (i.e., 4000 tons per year versus 3800 tons per year). No specific source of this discrepancy could be identified.
Another potentially significant reporting problem was identified at a third facility. For this one facility, hand calculations verified that the calculation module of WINCEIS produced reasonable results. However, available hardcopy data records from the facility did not match those pulled from the TNRCC database that were reportedly submitted to the TNRCC using the electronic reporting module of the software. Due to site-specific personnel changes and corporate restructuring, it is not possible to fully investigate the cause of this error. TNRCC staff and the facility’s operations staff have worked cooperatively to attempt to understand the discrepancies, which include both missing sources and differences in reported versus calculated emissions. At this time, it is not clear whether the source of the problem is a bug in the interface between the calculation and reporting software or human error in the application of the software. As noted previously, four or five of the eight facilities visited used the WINCEIS electronic software for reporting emissions to the TNRCC. However, only one of them also used the WINCEIS electronic software for calculating emissions, and this is the facility with the discrepancies.

Current emission inventory reporting requirements do not stipulate the documentation of potentially significant sources of temporal variability in emissions. While the annual emission totals may accurately reflect the sum of the emissions estimates, the actual emissions at any given moment could be substantially different than the annual emissions divided by 365 days and spread over 24 hours.

2.1.5 Quality Assurance Methods

A general finding is that facilities that maintain internal-use, systematic, plant-specific guidance documents of emissions estimation procedures tend to have higher quality emission inventories. This is particularly true for NOx emissions reported from continuous emissions monitors (CEMs). The site visits show clearly that industry is attempting to adhere to TNRCC emission inventory guidance, but errors are being introduced in the inventory process. Once introduced, errors are not being caught due, in part, to a lack of quality control at the reporting step. One key finding for quality control (QC) is that, in general, QC checks are insufficient in the reporting step between the facilities and TNRCC. We understand that TNRCC reports back to each facility after each inventory submission and relies on the facility to confirm the accuracy of the “official” records. However, it appears that this “loop” is not always completed.

2.2 SUMMARY OF FINDINGS

At this time, it is not possible to quantify the full extent of emission uncertainties in the HSC, but some qualitative assessments can be made regarding the initial objectives of the overall study.

- Because of the relatively small number of omission errors found in the reporting process, we conclude that there should be reasonable confidence in the completeness of the existing TNRCC emission inventory database.
Regardless of the source of error, significant reporting errors at one of the eight facilities suggest only modest confidence in the accuracy of the reported emissions in the TNRCC database.

On-site observations reveal that existing EPA emission inventory methods do not reflect local conditions and are not likely to produce accurate emission estimates.

3. RECOMMENDATIONS

The facilities that voluntarily participated in this study should work with TNRCC to correct any discrepancies identified. In addition, it is likely that similar discrepancies occur at similar industrial facilities. Thus, we suggest that TNRCC conduct a thorough review of its emissions database, focusing on the types of discrepancies identified during the ground truth exercise. Although the results from only eight facilities cannot provide conclusive evidence, real variations observed at these facilities, as well as reporting errors, could be used to develop a number of scenarios for use as modeling sensitivity runs. Sensitivity scenarios that account for increases in magnitude, alternative temporal allocations, and speciation to account for errors and increased emissions rates (from inaccurate methods or real temporal variations, such as upsets and maintenance) should be considered.

As a product of our visits to facilities and reviews of emissions data, we have developed several specific recommendations for consideration by TNRCC and industry representatives. The objective of these recommendations is to improve the quality of emissions estimates and the modeling inventory. The recommendations are aimed at (1) improving procedures for developing emissions estimates, (2) improving modeling inventories, and (3) remedying recurrent and/or recognized issues with the emission inventory data. Some recommendations could be implemented by TNRCC or industry alone, but some are best accomplished as a cooperative effort.

3.1 RECOMMENDATIONS FOR TNRCC

3.1.1 Upgrade and Improve Emissions Estimation Guidance

TNRCC has developed a series of guidance documents for industries to use in estimating emissions and preparing air quality permits. In addition, TNRCC periodically improves and upgrades the guidance documents. It is recommended that TRNCC continue this effort, especially for emissions sources that are common to many facilities and are associated with large, highly or unpredictably variable, and/or uncertain emissions estimates. Examples of such emissions sources are listed below. Some estimation methodology issues exist for several of these emissions source categories (marked with an asterisk, *) and are discussed in the following subsections. We recommend that TNRCC work with the EPA and others to improve emission methods for the following sources:
Flares present a difficult issue. They are one of the largest and most variable emissions source types for most of the plants that we visited. A critical question when determining emissions for flares is how to determine the actual, real-world destruction and removal efficiencies. On the basis of available information, TNRCC guidance delineates the selection of appropriate efficiencies for the purposes of emissions calculations. TNRCC guides facilities to select flare efficiencies from 98% to 99.5%, depending on chemical composition and operating parameters. However, the estimation guidance for flares is only as good as available manufacturer’s and research data. It is difficult to determine with great accuracy the destruction efficiency for a flare. In the range from 98% to 99.5% efficiency, even a small uncertainty in the decimal place represents a large uncertainty in the emissions estimate. For example, if a flare’s efficiency declines from 99.5% to 99.0%, VOC emissions double for that flare. Given the lack of available research data, there is no immediate solution to this problem. However, it is an important source of uncertainty in the inventory and should be a research priority if funding becomes available.

A simpler issue to address for flares is occasional confusion or inconsistency in the application of TNRCC guidance to select appropriate destruction efficiencies (i.e., 98% vs. 99% or 99.5 %). There are some possible means of remedying this potential problem:

(a) Provide clarifications in the guidance document. Some improvements could be made by providing quantitative definitions for the phrases “not difficult to combust” and “excessive variability in the volumetric flow”. The document could also include a discussion of whether different efficiencies could be applied to the components of the flare feed stream. For example, a flare that consumes a feed composed of 90% by weight C2 hydrocarbons and 10% C4 hydrocarbons might be considered to have an efficiency that is calculated as the weighted average of the efficiencies provided by TNRCC’s guidance as follows:

\[
(0.9 \times 99\% \text{ efficiency}) + (0.1 \times 98\% \text{ efficiency}) = 98.9\%
\]

(b) Perform QA review of selected control efficiencies. TNRCC staff could spot-check the control efficiency selection bases for one to three flares at each facility. This would likely reveal whether the TNRCC guidance was applied correctly by a particular facility.
The final point we note for flares is that some variability existed between facilities in their emissions estimation methods for VOCs. Facilities that operated fairly closely to their operating permit levels also tended to use detailed tracking or logging systems to produce accurate, real-time estimates of the compositions of flare feed gases. These real-time compositions could be applied to continuous volumetric flow data in order to produce the most accurate estimates and speciations possible for VOCs. Facilities with extra capacity in their operating permits had a greater tendency to estimate emissions conservatively and over-report VOC emissions.

**Fugitives**

Similar to flares, fugitives also present a difficult problem. Fugitive VOC emissions are estimated to be large but are very difficult to measure directly. All the plants we visited employed consistent leak detection and repair programs—whether performed by on-site personnel or specialty contractors—and applied consistent emissions estimation equations. Facilities varied only in the types and complexities of their database systems, which are used to track discovered leaks, generate emissions estimates, and apply VOC speciation profiles. Several complex facilities used their database systems to apply product stream-specific VOC speciation profiles to individual leaks. While systems have been put in place that produce reasonably precise emission estimates for fugitives, it is not clear how accurate or representative these emissions are of real-world conditions.

**Cooling Towers**

The most facility-to-facility variability in emissions estimation methods was observed for cooling towers. Several methods were used to estimate VOC emissions, including (1) the El Paso Method, (2) water analyses from a sampling point upstream of the cooling tower, (3) water analyses at upstream and downstream points (with a difference calculation), and (4) the use of emission factors from the EPA’s AP-42 Guidance Document. It is very difficult to collect and accurately analyze field samples of water with entrained or dissolved VOC without allowing any exposure to the atmosphere. Given this difficulty, the mechanics of the El Paso Method appear to be the most suitable for the particular problem of determining VOC concentrations in cooling tower inlet water. The El Paso Method could potentially be improved through one or more of the following means:

- Determine appropriate methods to collect and route cooling tower inlet water through the El Paso Method apparatus. Verify that the sampling point—top, bottom, side, or center of flow—has no effect on the results.

- Theoretically verify that the residence time in the El Paso apparatus is sufficiently long to completely volatilize all of the VOC species of interest at the specific plant. If this is the case, the VOC concentrations in the vapor space and water can be determined by simple mass balance calculations.

- Verify the speciation profile, VOC molecular weight, and total VOC emissions estimates by collecting canister samples in parallel with the OVA “sniffer”. Canister samples can be somewhat difficult to collect and analyze for a humid sample, but the problems can be overcome through careful techniques and the selection of appropriate drying materials.
Loading and Unloading Operations

Generally, plants use the methods that are described in EPA’s AP-42 guidance document, with adjustments to account for vapor recovery and routing to flare. However, our perception is that emissions from loading and unloading operations are highly variable from day to day and, because the operations require human intervention, the emissions control procedures are potentially subject to human error. We recommend developing a small-scale study—perhaps through a limited survey—to collect data to represent typical, short-term conditions for loading and unloading (e.g., number of tank cars/trucks on site over a period of several days, typical length of loading/unloading time, and length of time sitting on property).

Other Emissions Sources

Facilities tended to estimate emissions for the remainder of the emissions source types (listed below) consistently from facility to facility. In addition, emissions from these types of sources tend to vary in a predictable or obvious manner with time because they are closely tied with production rates; monitored through CEMS; and unlikely to experience undetected problems or malfunctions that would lead to changed emission rates.

- Boilers, heaters, and furnaces
- Turbines, engines, and compressors
- Incinerators
- Wastewater treatment systems
- Chemical or petroleum storage tanks

Although a low-priority problem, one common issue that may arise with the emissions estimation methodologies for these types of sources is representativeness of stack test data. Stack tests are usually performed at high-load operating conditions, which could be non-representative of normal operating emissions. We considered this to be a lower priority problem than those discussed in greater detail above because it seems unlikely to affect emission rates dramatically (e.g., by more than 25%).

3.1.2 Use Temporal Data Collected by TNRCC Regional Offices

Our understanding is that facilities provide reports of short-duration upset conditions to TNRCC regional offices to meet “Reportable Quantity” (RQ) requirements and that these upset data are time-averaged at some point before they are integrated into the ozone modeling inventory. This time averaging would dramatically dilute the effects of upsets on ozone formation. We recommend that the TNRCC make use of the time-specific data that industrial facilities currently report to TNRCC regional offices, which include time, date, duration, and total emissions for each upset occurrence. We understand that this will require several improvements to the system, such as expanding the regional offices’ capacity to electronically process data, update emissions estimates with more accurate revisions when they are provided at a later time, and transmit the data to the TNRCC Emission Inventory or Modeling sections.
3.2 RECOMMENDATION FOR INDUSTRY

Our investigation showed that facilities that employed SOPs facilitated higher quality emission inventories. Therefore, we recommend that all facilities develop and maintain facility-specific emissions estimation guidance document or standard operating procedures (SOP). The SOP documents seemed to help facilities (a) develop a continuous history of institutional knowledge about their facilities and their emission inventories, (b) create organized and complete internal filing systems, and (c) recognize QA/QC problems with the emission inventory more quickly.

In addition, we recommend that facility operations staff follow through with their stated plans to make it a priority to work with TNRCC to rectify all of the discrepancies uncovered by the ground truth investigations.

3.3 JOINT RECOMMENDATIONS FOR INDUSTRY AND TNRCC

3.3.1 Additional Data Quality Assurance Steps

TNRCC has established a comprehensive emission inventory reporting and data archive system. To further enhance the confidence in the data archive, we recommend that additional quality assurance steps be taken:

- Check sums of reported VOC species against reported total VOCs.
- Use GIS as a QA checking tool to identify large spatial discrepancies.
- Close the QA “loop”—that is, put in place a mechanism to ensure that facilities check their data as archived by the TNRCC, by comparing their records with the emissions report letter that TNRCC routinely sends.

3.3.2 Emissions Specialist Training and/or Certification Program

The site visits show clearly that industry is attempting to adhere to TNRCC emission inventory guidance, but errors are still being introduced in the inventory process. Once introduced, errors are not being caught due, in part, to a lack of quality control at the reporting step. In addition to the enhanced quality assurance checks recommended above, we recommend that TNRCC consider instituting an emissions inventory training and/or certification program. The program should cover both emission estimation methods for industrial sources and procedures for reporting emissions to the TNRCC. Course attendees might include facility operations staff as well as private contractors (who are currently performing emissions calculations for some facilities).