VOLUME VI: Chapter 3

GENERAL QA/QC METHODS

Final Report

June 1997

DISCLAIMER

As the Environmental Protection Agency has indicated in Emission Inventory Improvement Program (EIIP) documents, the choice of methods to be used to estimate emissions depends on how the estimates will be used and the degree of accuracy required. Methods using site-specific data are preferred over other methods. These documents are non-binding guidance and not rules. EPA, the States, and others retain the discretion to employ or to require other approaches that meet the requirements of the applicable statutory or regulatory requirements in individual circumstances.

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1

INTRODUCTION TO METHODS

This chapter is a compilation of methods that can be used to implement a quality assurance/quality control (QA/QC) program, and should be consulted when preparing the quality assurance plan (QAP) at the beginning of inventory development (see Chapter 2 of this volume). The QA/QC methods to be employed should be determined and specified in the QAP. The data quality objectives (DQOs) and the inventory level will determine which methods and the number of different methods that are adequate for a given inventory. Such methods need not be limited to those described in this document; in fact, the inventory preparer is encouraged to develop or identify new tools or methods as needed to meet the DQOs set for the inventory.

The QA/QC methods described in this chapter are classified into the following general categories based on the type of activity involved:

- Reality checks;

- Peer review;

- Sample calculations;

- Computerized checks;

- Sensitivity analysis;

- Statistical checks;

- Independent audits; and

- Emissions estimation validation.

These methods are presented in order of increasing complexity. Each method has specific functions, although methods can be combined to cover a wider range of functions. The more complex and/or labor-intensive methods fulfill more than one function. Table 3.1-1 shows the primary function(s) of each type of method.

Any one of these methods by itself does not constitute a complete QA/QC program. Table 3.1-2 shows the minimum combination of methods recommended by the Emission Inventory Improvement Program (EIIP) for inventories at each level (see Chapter 2,

TABLE 3.1-1

PRIMARY QA/QC FUNCTIONS OF GENERAL TYPES OF METHODS

Method	Ensure Reasonableness of Emissions, Data	Ensure Validity of Assumptions, Methods	Ensure Mathematical Correctness	Ensure Valid Data Were Used	Optimize QA/QC Efforts	Ensure Proper Implementation of QA/QC Program	Assess Accuracy of Estimates
Reality checks	X						
Peer review	X	X					
Sample calculations			X	X			
Computerized checks	X		X	X			
Sensitivity analysis		X			X		
Statistical checks	X		X				
Independent audits	X	X	X	X	X	X	
Emissions estimation validation	X	X					X

Section 1 of this volume). Two of the methods--computerized checks and statistical checks--are not included in Table 3.1-2 because their function can largely be achieved using other methods. Moreover, these two general types of methods require specialized tools and/or expertise that may not be available to everyone. However, computerized and statistical checks can and should be used to the extent possible. They usually allow the processing of greater amounts of data than manual methods, and also reduce the chance of human error (on the part of the reviewer). Emissions estimation validation is also not listed in Table 3.1-2 because it requires resources and expertise that are beyond the capabilities of many organizations; however, these methods are very valuable as QA/QC tools and can be used to enhance the value of a QA program.

The methods presented in this chapter are designed to minimize the errors that can occur when developing an emission inventory. These errors can be of two types: procedural and technical.

Procedural errors result from unclear and ineffective management, inadequately trained staff, improper planning, lack of adequate QA, lack of data tracking and handling protocols, and other problems related to how the work gets done.

Technical errors are directly related to the methods and technologies used to develop emission estimates. They may result from:

- *Incorrect use of spreadsheets and databases*: Certain types of errors are solely a consequence of the mechanics of databases and spreadsheets. For example, an inadvertent reference to the wrong cell in a spreadsheet or retrieval of information from the wrong storage location in a database is very difficult to detect if the information in the erroneous data source and in the desired data source are similar.

- *Mathematical errors*: These types of errors can occur in hand calculations or in spreadsheets. They include the use of incorrect conversion factors, mismatched units in the emission factor and activity parameters, incorrect constants, and arithmetic errors.

- *Incorrect use of emission inventory software*: Software for calculating emissions is generally designed to minimize errors; however, it is possible to incorrectly calculate emissions if the user does not follow the instructions.

- *Use of incorrect data*: This covers a wide range of errors including the use of out-of-date data, inappropriate surrogate data, and data that do not correctly match the source category definition. This applies to both activity data and emission factors.

TABLE 3.1-2

MINIMUM RECOMMENDED QA/QC ACTIVITIES BY INVENTORY CATEGORY

Method	Level 1	Level 2	Level 3	Level 4
Reality checks	✓	✓	✓	✓
Peer review	✓	✓	✓	✓
Sample calculations	✓	✓	✓	
Sensitivity analysis	✓	✓[a]		
Independent audits	✓	✓[a]		

[a] Level 2 may include fewer audits and/or different types of sensitivity analyses and audits than Level 1.

- *Use of incorrect methodology and/or assumptions*: Methodology is defined to include both computer models (e.g., MOBILE5b) and prescribed methodology (e.g., the use of gasoline throughput in a county and an emission factor to calculate evaporative emissions from gasoline dispensing is a type of model). This category covers just about any other errors not included in the first four error types.

- *Failure to include all sources*: This addresses inventory completeness. For a point source inventory, the omission of some emission units makes an inventory incomplete. For a regional inventory, this also covers failure to include entire source categories.

- *Double-counting emissions*: Double-counting of emissions between area and point source inventories is a technical error that results in an overestimate of the emissions reported.

This chapter primarily covers QA/QC methods that address technical errors, although the section on independent audits includes methods for reducing procedural errors. Other chapters of this volume (*Planning and Documentation, Model QA Plan*) as well as U.S. Environmental Protection Agency (EPA) guidance (EPA, 1988; EPA, 1989) address procedural QA activities. In general, avoiding or minimizing procedural errors will reduce the likelihood of technical errors.

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2

REALITY CHECKS

QUICK REVIEW

Definition:	An assessment of an emission estimate or data designed to answer the question, "Does this make sense?"
Objective:	Ensure that the value being checked is not wildly improbable, or that it is within a specified range or limit that is considered reasonable.
Optimal usage:	Anywhere and everywhere throughout the inventory development process. This method provides the quickest and easiest means of spotting large mistakes before the process has advanced very far.
Minimum expertise required:	Moderate. Although relatively inexperienced inventory developers can be trained to use this method (provided they are given some guidance and documents to use as a reference), personnel with some experience with emission inventories will be the most efficient and effective.
Advantages:	Quick, easy.
Limitations:	(1) It is possible that a value is "reasonable" but is still wrong, (2) it is possible that a value appears unreasonable but is still right, (3) the method does not give any insight into the source of an error, and (4) the method is only reliable if a valid point of reference is available.

2.1 OVERVIEW OF METHOD

The reality check is probably the most commonly used QA/QC method. It can be particularly useful for catching large errors early in the process. This check is a form of assessment to answer the questions "Is this number reasonable? Does it make sense?" However, it is important to remember that an estimate can appear to be wrong (that is, higher or lower than expected) but still be right. The opposite is also true--a value can look reasonable when it is actually incorrect. For these reasons, the reality check is never used as the sole criterion of quality.

To be able to answer the above questions, some notion of a reasonable value must be known. If the questioner is knowledgeable about emission inventories, he or she may not need an external reference to answer the question. However, if a standard reference value is available, the preferred method for a reality check is to use an external reference value.

Other types of reality checks include comparing the value to its equivalent value from a previous or alternative inventory or database. Another check might compare the estimated emissions to those calculated for the same category in a nearby or similar region. Table 3.2-1 summarizes the preferred and alternative methods for performing reality checks.

TABLE 3.2-1

REALITY CHECKS: PREFERRED AND ALTERNATIVE METHODS

Method	Procedure
Preferred	Compare data or estimate to a standard reference value.
Alternative 1	Compare data or estimate to a value from a previous or alternative inventory (or database) for the same region.
Alternative 2	Compare data to values used for other regions.
Alternative 3	Use expert or engineering judgment to assess the reasonableness of the values.
Alternative 4	Compare estimates for similar categories within the same inventory.

2.2 COMPARISON TO REFERENCE VALUE

This method can be used to assess the reasonableness of the emission estimates or of the data used to calculate those estimates. For a Level 1 or 2 inventory, this method should be used as much as possible. For example, emissions for many area source categories are estimated using population, employment, or other readily available surrogates for emissive activities. Generally, the preferred area source estimation method is to use local survey data. A good reality check for these locally obtained values is to compare them to some of the statistics generated by federal (or other) agencies.

Standard references for commonly used data are shown in Table 3.2-2. These data sources are often used as a source of activity data for area source calculations; in these cases, an alternative reference for reality checks is needed.

TABLE 3.2-2

STANDARD REFERENCES FOR COMMONLY USED DATA (ANNUAL UPDATES)

Reference	Types of Data	Resolution
U.S. Dept. of Commerce, Bureau of the Census (year). *19__ Census of Population and Housing, Summary Population and Housing Characteristics*, (state, year) CPH-1-34. Washington, DC.[a]	Population, number of housing units by type	Townships, other sub-county units
U.S. Department of Commerce, Bureau of the Census (year). *County Business Patterns* - (state, year). Washington, DC.[a]	Employment by Standard Industrial Classification (SIC) code and size of establishments	County level
U.S. Dept. of Commerce, Bureau of the Census (year). *19__ Census of Manufacturers*. Geographic Series MC87-A1 to -51. Washington, DC.[a]	Employment, hours worked, value of shipments and other data by SIC code group	County and state level
U.S. Department of Commerce (year). *Statistical Abstract of the United States*, (year). Washington, DC.[a]	Wide variety of useful data: economics, population characteristics, energy use, industrial production	National, regional; some state level data

TABLE 3.2-2

CONTINUED

Reference	Types of Data	Resolution
U.S. Department of Energy, (year). *State Energy Data Report Consumption Estimates, 1960-year*, Energy Information Administration, SOW/EIA-0124(xx). Washington, DC.	Fossil fuel consumption by sector	State level
U.S. Department of Transportation, (year). *Highway Statistics* (year). Federal Highway Administration, Washington, DC.	Vehicle miles travelled, onroad and offroad fuel consumption	State level
U.S. Environmental Protection Agency, 1993. *Regional Interim Emission Inventories (1987-1991), Volume 1: Development Methodologies*, EPA-454/R-93-021a. Research Triangle Park, NC.	Emissions of criteria pollutants	County level
U.S. Environmental Protection Agency, 1994. *National Air Pollutant Emissions Trends, 1990-1993*. EPA-454/R-94-027. Research Triangle Park, NC.	Emissions of criteria pollutants	National

[a] Data based on most recent census; therefore, accuracy decreases each year beyond the most recent census.

2.3 COMPARISON TO OTHER REGIONS

Another type of reality check is to compare results to those from different regions. A region that is very similar may be chosen with the expectation of similar emission estimates. An alternative approach is to contrast regions known to be different with the expectation that one region will have higher emissions than the other.

When using this approach, care should be taken to consider (and possibly remove) any effects that make comparisons unequal. For example, two counties may be similar in terms of type of industry and community characteristics, but very different in size. Therefore,

comparing emissions on a per capita, per employment, or other consistent basis should be considered.

Figure 3.2-1 shows an example of a graphical comparison of daily volatile organic compound (VOC) emissions on a per-capita basis in three neighboring regions: the portion (multiple counties) of a large Metropolitan Statistical Area (MSA) in State 1, the portion of the MSA in State 2, and an adjacent county in State 1 that is more similar to the State 2 MSA region with respect to population density, road types, and industrial development. The expectation was that the State 1 adjacent county and State 2 MSA region would have more similar per capita emissions than the densely populated State 1 MSA region. The onroad emissions are as expected: vehicle miles travelled (VMT) per capita is lower on average in densely populated urban areas. However, nonroad emissions for these three areas should be more similar on a per-capita basis. The discrepancy in area source emissions was also cause for concern because both inventories were known to be complete in their coverage of sources. This reality check suggested that the data and methods used for nonroad and area source emissions need further investigating (this example came from early draft inventories of an actual urban area; the difference in nonroad emissions were found to be the result of inventory developers from the various regions using different technical approaches to calculate emissions. The area source differences were found to be partly due to differences in the types of sources and to differences in the level of controls in place).

2.4 COMPARISON TO OTHER CATEGORIES

Comparing categories within an inventory to other categories within the same inventory is another type of reality check. For example, nitrogen oxides (NO_x) emissions from utility boilers could be compared to those from industrial space heaters (point sources). Emissions from solvent usage from different area source categories could also be compared relative to the anticipated level of solvent usage or prevalence of controls. In both examples one may expect to find dissimilar emission estimates; the degree of dissimilarity to expect serves as the reality check and is dependent on the experience of the inventory developer.

Global checking of this type could help to quickly identify emissions estimates that may be erroneous. Additional checking is needed when data are suspected to be unreasonable. One must remember that reality checking is merely a screening process; therefore, it should never be used solely as a means of determining data quality.
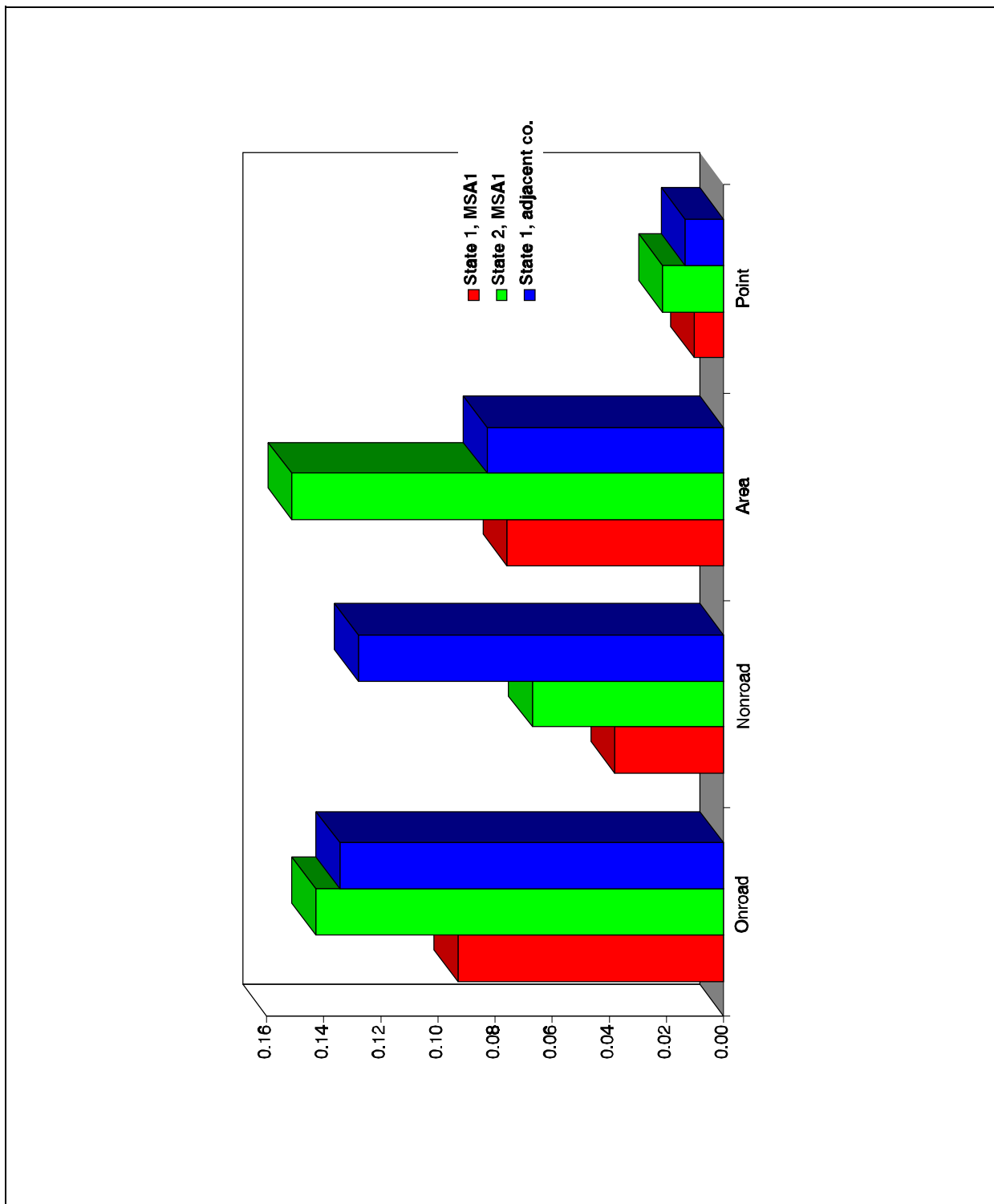
FIGURE 3.2-1. COMPARISON OF PER CAPITA DAILY VOC EMISSIONS

3
PEER REVIEW

QUICK REVIEW

Definition:	An independent review of calculations, assumptions, and/or documentation by a knowledgeable expert in the technical field. This is generally accomplished by reading or reviewing documentation, but may not include rigorous certification of data or references such as might be done in a technical audit (see Section 8 of this chapter, "Independent Audits").
Objective:	Ensure that assumptions and procedures used are reasonable and meet expectations as judged by persons knowledgeable in a specific field.
Optimal usage:	At critical points where: (1) information is organized in a manner amenable to review, (2) before critical decisions or commitment of large amounts of resources must be made, and (3) when the document, inventory, or database is completed, but prior to its release.
Minimum expertise required:	Moderate to high. Although the term "peer" implies equality, the most effective peer review is often done by someone with a high level of expertise. At a minimum, the expertise of the reviewer should be equivalent to the expertise required to manage the aspect of the inventory development activities from which the data to be reviewed were generated.
Advantages:	Usually not a labor-intensive effort; very flexible.
Limitations:	(1) Peer review is a form of reality check (and therefore has similar limitations), (2) the review is often general and does not check accuracy or quality of original data, and (3) for a large and/or complex inventory, it is very easy for a peer reviewer to miss errors.

3.1 OVERVIEW OF METHOD

The peer review process is very flexible and generally does not require specific tools; however, the use of checklists or review forms, which also provide a means of documenting QA/QC procedures, is strongly encouraged. If checklists are not used, the peer reviewer should provide feedback in the form of written comments. In some cases, the peer

reviewer's comments may be transmitted verbally, however, the inventory developer should document when the review took place, the major points or items of discussion, and steps that will be taken to address the comments. Table 3.3-1 summarizes the preferred and alternative methods.

TABLE 3.3-1

PEER REVIEW: PREFERRED AND ALTERNATIVE METHODS

Method	Procedure
Preferred	Use of a checklist showing elements to be covered by the review. Provides a guide for the peer reviewer and can be tailored to fit specific situation.
Alternative 1	Written comments by reviewer identifying issues noted.
Alternative 2	Written notes summarizing reviewer's comments identifying issues noted by reviewer as told to author of notes.

At a minimum (i.e., for a Level 4 inventory review), a peer reviewer will perform some reality checks. A more in-depth review will include some checks of the calculations and verification that correct data and emission factors were used. Access to original data and reports is required to conduct in-depth reviews. The extent of the review required will depend on other QA/QC activities, the DQOs, and the inventory category (Levels 1-4; see Chapter 2 of this volume). If adequate calculation checks and/or data verification are being conducted as part of the QA program, the peer reviewer may be asked to concentrate on the validity of the methods and assumptions.

3.2 CHECKLISTS

The peer reviewer should have a clear understanding of what he or she is expected to do. A checklist is the most expedient way to accomplish this. The completed checklist also provides documentation that the specified QA program procedures were followed. The peer review checklist is usually prepared by the Inventory Development Manager and the task leaders, with the assistance of the QA Coordinator and peer reviewer. Examples of checklists that can be used for peer review are discussed below.

3.2.1 EPA's LEVEL I AND LEVEL II CHECKLISTS

The EPA's Level I/Level II checklists were used to review the 1990 base year State Implementation Plan (SIP) inventories. Many of the items are specific to SIP inventories and may not apply to other types of inventories. An important limitation of the Level I checklist is that it only deals with procedures or methods used to calculate emissions--it does not address the validity of the assumptions or data used in the calculations. The Level II checklist is more detailed, but also fails to fully address some of these important issues.

A complete copy of the Level I and Level II checklists and guidance for their use is found in *Quality Review Guidelines for 1990 Base Year Emission Inventories* (EPA-450/4-91-022)(EPA, 1991a). An automated version of the checklists is available through the Clearinghouse for Inventories and Emission Factors (CHIEF) bulletin board.

3.2.2 CHICAGO AREA SOURCE TOXICS INVENTORY

The example checklist shown in Figure 3.3-1 was designed for a detailed peer review of individual area source categories. The reviewer is asked to answer nine specific questions. The QA program for this inventory included extensive QC checks of the calculations and a procedural audit, but no technical audit was planned. Therefore, a thorough peer review that included some data verification and calculation checks was used (see Section 4, "Sample Calculations," of this chapter).

This checklist includes a place ("QC review") for the peer reviewer to sign. The QA review signature space is provided for the procedural audit. The QA auditor signs to show that he or she reviewed the form as part of the audit (see Section 8, "Independent Audits," of this chapter). The auditor's signature indicates a check was performed to determine whether approved procedures were followed and whether problems identified were resolved.

3.3 PEER REVIEWER REPORTS

These reports may take the form of a memorandum or other less formal report. Providing a form for the reviewer's comments will facilitate the production of this report. The example shown as Figure 3.3-2 is a reviewer's comments on calculations of VOC losses from gasoline distribution. It is a good example of a peer review because the strengths as well as the weaknesses are described. The reviewer is also very clear about what he did and did not check. This was a very thorough peer review; note the suggestions for improving the presentation of the data (items 3 and 5). This emphasizes the importance of clear and thorough documentation for QA/QC. Finally, the reviewer makes recommendations on how to improve the estimates.

CHICAGO AREA SOURCE TOXICS INVENTORY
Source Category Review

CATEGORY DESCRIPTION:

INVENTORY REGIONS COVERED:

NAME (person responsible for calculations): _____

Signature (QC Review) _____   Date _____

Signature (QA Review) _____   Date _____

Checklist	YES	NO	Could Not Be Determined
1. Were all speciation profiles clearly referenced?			
2. Were correct emission factors used?			
3. Were sources of activity data clearly referenced?			
4. Were correct activity data used?			
5. Were annual emissions correctly adjusted from daily estimates?			
6. Were all calculations documented?			
7. Are calculations correct?			
8. Were applicable regulations cited?			
If so, were RE and RP correctly applied?			
9. Were adjustments made to account for any excluded VOCs?			

The following problems need to be corrected:

_____

_____

_____

_____

ACTION TAKEN:

_____

_____

FIGURE 3.3-1. EXAMPLE OF A PEER REVIEW CHECKLIST

QC-1 Comments on the NY SIP Inventory Gasoline Marketing Area Sources

9/16/92

GDRives

1. Emission factors are in general agreement with AP-42. Include tank truck in transit loss emission factors in Table 2 of the documentation. Emission factors could be refined a little bit to reflect typical gasoline RVP values and summer temperatures. Note that the state has a gasoline RVP restriction (<9 psia) during the ozone season (NY Rules Subpart 225-3, page 461:0593 BNR). Normal daily mean temperature for NY is probably closer to 70° F for the ozone season than 60. If you plan to refine emission factors any, I would probably select the midpoint of the range for transit losses since they have a tank truck tightness testing and certification program.

2. Assumptions on filling methods are outlined nicely for the NY metro area, what filling assumptions were used for the other areas? I recommend expanding Table 1 to address all areas.

3. Table 1 and Table 3 are not parallel which makes it difficult to review. I'd recommend presenting all information in the same sequence (i.e., county and area orders)

4. Table 3. Don't include NOx and CO for this source since they will just remain blank. Instead, you could present annual gasoline throughput by county, and assumptions on penetration of Stage I and II controls. This would provide all the activity data necessary to independently perform calculations.

5. Table 3. A little bit of clarification on Table 3 would help the review. At first glance, the columns don't add up correctly. With a more detailed look, you can figure it out but it leads to confusion. For example, NY Metro Area appears to have 11 components for a total of 13,192 tpy. However, "NYC Sum" appears to be a subtotal of the same group and should not be included in the totals, by the indention it appears to be just another county. Why don't we put NYC sum under the subtotal row?

6. Calculations look real good for NY area including the application of rule effectiveness for loading operations. I've checked a couple of the counties, and they are spot on. I can't independently verify the calcs for other areas, why did we use 90% rule effectiveness for loading?

7. I would have probably applied rule effectiveness when calculating emissions from submerged filling as well as vapor balance. I understand that you have already discussed with EPA and have reached consensus.

FIGURE 3.3-2. EXAMPLE OF WRITTEN PEER REVIEW REPORT

8.   I reviewed all of the county-specific gasoline throughput values to ensure that the data were correctly transcribed from the hard-copy supplied by the state energy office to our spreadsheets. With the exception of Tiago County, all matched correctly. Note that Tiago County should be 25460 instead of 25450.

9.   Have we performed any sanity checks on these gasoline consumption data? A couple of checks would be to calculate gal/person, gal/VMT, and gal/registered vehicle for each of the NY counties. Then calculate average and standard deviation for each. Any counties outside of 2 std deviations from the mean deserve to be investigated.

10.   I like the inclusion of supporting materials with the writeup. I hope that the plan is to submit this inventory with the documentation.

11.   Add dates and document numbers to the references, where appropriate.

FIGURE 3.3-2. CONTINUED

4

SAMPLE CALCULATIONS

QUICK REVIEW

Definition:	Verification of values calculated using spreadsheets, models, or hand calculations by *replicating* the calculations by hand or electronically; a subset or sample of each type of calculation is checked.
Objective:	Ensure that calculations are done correctly, minimizing mathematical and spreadsheet errors.
Optimal usage:	Should be used extensively and frequently as a QC tool; also used as part of a technical audit.
Minimum expertise required:	Low to moderate. Replication of calculations can be done by anyone capable of doing the work (i.e., some expertise in inventory development recommended).
Advantages:	(1) Most reliable way of detecting computational errors, (2) can be done by anyone involved in inventory development, and (3) does not require expensive or complicated tools (only pen and paper).
Limitations:	(1) Does not ensure that approach and assumptions used are correct, and (2) is labor-intensive.

4.1 OVERVIEW OF METHOD

Replication of calculations is one of the most basic quantitative QA/QC methods available. It should be used by the author of the original calculations as a self-check, by the person performing QC checks, and as part of any QA audit.

Self-checking using manual or electronic calculations is strongly encouraged when spreadsheets are used to calculate values. Each author should be encouraged to include an example calculation replicating one complete set of calculations on his spreadsheet or as an attachment to help facilitate the review of the technical approach and identify errors. If the original calculations are done by hand, replication by the author may still be useful.

The most common usage of this method is by the person conducting the QC check. The preferred QC method is to replicate one complete set of calculations from beginning to end. In addition to verifying the mathematical correctness of the calculation, the values used should also be verified. For example, use of the correct emission factor should be checked. If the original calculations are in a spreadsheet, spot checks of the remaining values (assuming the same equations are being used repetitively) is sufficient. The percentage of calculations that should be checked will depend on several factors, including:

- The complexity of the calculations;

- The DQOs for the inventory; and

- The error rate encountered.

The error rate is determined during the QA/QC process. If a large number of errors is being detected, the number of checks should be increased, although not necessarily on a given version of the spreadsheet. For example, during the initial check, several errors may be found. The person conducting the QC check may stop after working through one set of calculations and send it back to the author for revision. In the second review, the original calculation is rechecked and found to be correct. The person conducting the QC check then proceeds to check another set of calculations; if no errors are found, he or she may spot check a few more values before approving the calculations (see Section 7, "Statistical Checks," for more discussion on statistical QC procedures).

The procedures for determining the number of calculations to be checked and the number of iterations required before the calculations are approved are a function of the DQOs and should be specified in the QA plan. Ensuring that the specified QC procedures are followed is the responsibility of the QA Coordinator.

In addition to checking the arithmetic used, the proper conversion of all units should be verified. Units analysis may be done independently of the actual values.

Replication of calculations by hand (e.g., using pen, paper, and calculator) is the preferred method for checking calculations originally performed by hand or in a spreadsheet. Spreadsheets can be used as an alternative; however, they are not preferred as a QA technique because they introduce the possibility of other errors unique to spreadsheets. In certain situations, it may not be feasible to replicate calculations; for example, if emissions are generated by a model, the algorithm may either be unknown to the user or too complex to repeat by hand. A check would be to attempt to approximate the result using an alternative method; this is a more complex type of a reality check. Table 3.4-1 summarizes the preferred and alternative methods.

TABLE 3.4-1

CALCULATION CHECKS: PREFERRED AND ALTERNATIVE METHODS

Method	Procedure
Preferred	Hand replication of one complete set of calculations.
Alternative 1	Hand replication of most complex calculations.
Alternative 2	Hand calculation using a different method, attempting to approximate the result.

4.2 REPLICATION OF SPREADSHEET OR HAND CALCULATIONS

Figure 3.4-1A shows spreadsheet calculations of structure fire emissions for several counties. Figure 3.4-1B shows the original hand-calculated QC checks of one county's emissions. Note that the reviewer did *not* verify emissions of all counties; a reality check was used to check the others. Depending on the DQOs for the inventory, this level of checking may be adequate, particularly if combined with a spreadsheet audit (see Section 5.2.4, "Spreadsheet Auditing Functions").

4.3 REPLICATION OF COMPLEX CALCULATIONS

When a model or other software program is used to calculate emissions, hand replication of each type of calculation performed is the preferred method. However, if the calculations are very complex or cannot be duplicated easily, an alternative approach is to attempt to

STRUCTURAL FIRE EMISSIONS FOR OZONE SEASON

AUTHOR: M. Fauls
PREPARED: 9/10/92
PURPOSE: Prepare ozone season emission estimates of NOx, CO, and VOC from structure fires in New York Counties

CHECKED BY: _____
DATE: _____

New York Metropolitan Nonattainment Area O3 Season: Summary of Emissions From Structural Fires   SCC 28-10-030-000

	(a) Number of Fires (yearly)	(a) % of Fires in Ozone Season	(b) Tons Burned (yearly)	(c) Emission Factors (lb/ton) NOx	(c) CO	(c) VOC	(d) Activity (days/wk)	(e) NOx Emissions Annual (ton/yr)	(e) NOx Emissions Ozone Season (lbs/day)	(f) CO Emissions Annual (ton/yr)	(f) CO Emissions Ozone Season (lbs/day)	(g) VOC Emissions Annual (ton/yr)	(g) VOC Emissions Ozone Season (lbs/day)
New York Metropolitan Area													
Bronx	6775	24.3%	46070.00	1.4	60	11	7	32.2	170.4	1382.1	7301.1	253.4	1338.5
Kings	9245	24.3%	62866.00	1.4	60	11	7	44.0	232.5	1886.0	9962.9	345.8	1828.5
New York	7787	24.3%	52951.60	1.4	60	11	7	37.1	195.8	1588.5	8391.7	291.2	1538.5
Queens	4367	24.3%	29695.60	1.4	60	11	7	20.8	109.8	890.9	4708.1	163.3	862.8
Richmond	934	24.3%	6351.20	1.4	60	11	7	4.4	23.5	190.5	1006.5	34.9	184.5
Nassau	1094	25.6%	7439.20	1.4	60	11	7	5.2	29.0	223.2	1242.0	40.9	227.7
Suffolk	1313	26.2%	8928.40	1.4	60	11	7	6.2	35.6	287.9	1525.8	49.1	279.7
Westchester	2049	27.5%	13933.20	1.4	60	11	7	9.8	58.3	418.0	2498.9	76.6	458.1
Rockland	193	26.4%	1312.40	1.4	60	11	7	0.9	5.3	39.4	226.0	7.2	41.4
Orange	172	28.8%	1168.12	1.4	60	11	7	0.8	5.1	35.0	219.4	6.4	40.2
Total Structural Fire Emissions =								161.5	865.2	6921.5	37080.2	1268.9	6798.0

NOTES:

(a) Information supplied by NYSDEC Office of Fire Prevention and Control except for the five New York City boroughs. This information came fro the Fire Department of the City Of New York. FDNY Annual Report and Statistics–1991. Brooklyn, NY, p.65. Percentage of Fires in the Ozone Season for the five New York City boroughs was calculated using data provided by the Fire Department of the City of New York. FDNY Annual Report and Statistics–1990. Brooklyn, NY, p.58. Orange county apportionment based on the number of structure, ref. Orange County Memo, September 3,1992. Tompkins County information is derived from the county population times the statewide average number of fires per 1000 people, New York Department of State, Office of Fire Prevention and Control. Fire in New York 1990. Albany, NY, p.4.

(b) Tons Burned = (Yearly Number of Fires)*(Fuel Loading Factor)
The fuel loading factor is taken from the EPA Procedures Document, Section 4.8.4.
The value used in this inventory is 6.8 tons of material per fire.

(c) Emission factors are taken from the EPA Procedures Document, Section 4.8.4.

(d) Activity is taken from the EPA Procedures Document, Table 5.8-1.

(e) (Annual Emissions t/yr) = (Tons Burned) * (Emission Factor lbs/ton)/ (2000 lbs/ton)

(f) (Ozone Season Emissions lbs/day) = (Tons Burned) * (% of Fires in Ozone Season) * (Emission Factor lbs/ton)/(# of Days in the Ozone Season)

FIGURE 3.4-1A.   EXAMPLE SPREADSHEET CALCULATION

SIGNATURE _R. Peer_____ DATE _9/15/95_ CHECKED _WA_ DATE_____
PROJECT _Ozone inventory_ JOB NO. _____
SUBJECT _QC checks of "Structure Fires"_ SHEET _1_ OF _1_ SHEETS

Objective: Check calculations in STRUCTO3.XLS.

Largest (in terms of emissions) county was chosen - Kings.

(1) Annual emissions (tn/yr) = $\dfrac{\text{Tons burned/yr} \times \text{Factor (lb/ton)}}{2000 \text{ lb/ton}}$

$\begin{array}{l}\text{Annual} \\ \text{emissions} \\ \text{(t/yr)}\end{array} = \dfrac{62{,}866 \text{ tn/yr} \times 60 \text{ lbs CO/tn}}{2000 \text{ lb/tn}} = 1{,}885.98 \text{ t/yr}$

(2) Ozone season emissions (lbs/day) =

$\dfrac{(\text{tons burned/yr}) \times \left(\dfrac{\% \text{ Fires in O}_3 \text{ Season}}{100}\right) \times \text{Factor (lb/tn)}}{\# \text{ days in ozone season}}$

$= \dfrac{62{,}866 \text{ tn/yr} \times 0.243 \times 60}{92} = 9{,}962.89 \text{ lb/day}$

Conclusions:
- Kings Co. calculations verified by replication of CO emissions shown above, NOx and VOC were verified (but not shown).

- Other counties appear correct based on visual comparison of values.

- Documentation adequate, except number of days in ozone season not shown. Equation (f) should show division by 100.

FIGURE 3.4-1B. EXAMPLE OF HAND-CALCULATED CHECK OF SPREADSHEET RESULT

duplicate the result using an alternative calculation method.

The following example shows one approach to checking the calculations used in an emissions estimation software program. The Air Quality Utility Information System (AQUIS) (U.S. Air Force, 1994; Smith et al., 1995) is used by the U.S. Air Force, Air Combat Command, to estimate air emissions at a single site.

Note that this type of check only confirms that the mathematical calculations are performed as expected. Any data that are supplied by the software (e.g., conversion factors, emission factors) should also be verified and input data need to be checked (see Section 3, "Peer Review," Section 5, "Computerized Checks," and Section 8, "Independent Audits").

Figure 3.4-2 shows a hand-calculated check of the AQUIS algorithm for industrial reciprocating engine emissions (The original calculations were subsequently typed to give a neater presentation for a report). The input data used in both the program and the hand calculation are shown in Section I. The equation used by AQUIS (as reported in the AQUIS Algorithm Manual) is shown in Section II. Sample calculations are shown for three hazardous air pollutants and the results compared to the program output (The third page, not shown, contains a list of all pollutants calculated by AQUIS).

Although this level of checking for a program can require a significant amount of time, it is necessary. Furthermore, given that these programs are generally used many times over, the effort required to check the algorithms is relatively small.

CALCULATION SHEET

                                                                                  CALC. NO._2_

SIGNATURE_____J. Scientist_____ DATE__6/30/94_ CHECKED_R. Peer__ DATE_

7/13/94_____

PROJECT_____**Inventory Database QA**_____JOB NO._____

SUBJECT_____**Review of AQUIS Methodology**_____ SHEET__1__ OF__3__SHEETS

INTERNAL COMBUSTION GENERATORS

I.   Input Data:

        Type of Stationary Source = Industrial reciprocating engine
        Fuel = Diesel
        Rated Power = 201.2 hp
        Hourly Max Fuel Usage = 10.13 gal/hr
        Annual Average Fuel Usage = 1.6694×10^3 gal/yr
        Fuel Unit of Measure (fu) = gal

II.   Annual Emissions Calculation:

        AAUE = NPIE * HV * EF(P) * AU

        where:

                        AAUE =   Annual emissions from generators (lb/yr)

                        NPIE =   Number of identical pieces of equipment = 1

                        HV   =   Heating value of fuel = 137 (10^3 Btu/fu)
                              = 137×10^3 Btu/gal

                        EF(P) =   Emission factor for pollutant P (lb/10^6 Btu) for
                                        Type 2
                                        (from Table 3.2.1-4)

                        AU   =   Annual average quantity of fuel (10^3 fu/yr)
                              = 1.6694×10^3 gal/yr

        This is the Type 2 equation (one of three types), where type is a function of
engine design and pollutant.

FIGURE 3.4-2. EXAMPLE HAND-CALCULATED CHECK OF DATABASE ALGORITHM

CALCULATION SHEET

CALC. NO.__2__

SIGNATURE_____J. Scientist_____ DATE__6/30/94_ CHECKED R. Peer__ DATE_

7/13/94

PROJECT_____**Inventory Database QA**_____ JOB NO._____

SUBJECT_____**Review of AQUIS Methodology**_____ SHEET__1__ OF__3__SHEETS

A. For 1,3-Butadiene:

AAUE = $1 * 137 \times 10^3$ Btu/gal $* 3.91 \times 10^{-5}$ lb/10^6 Btu $* 1.6694 \times 10^3$ gal/yr

= 8.94×10^{-3} lb/yr 1,3-Butadiene

AQUIS Printout: AAUE = 0.009 lb/yr 1,3-Butadiene

B. For Benzene:

AAUE = $1 * 137 \times 10^3$ Btu/gal $* 9.33 \times 10^{-4}$ lb/10^6 Btu $* 1.6694 \times 10^3$ gal/yr

= 0.213 lb/yr Benzene

AQUIS Printout: AAUE = 2.213 lb/yr Benzene

C. For Naphthalene:

AAUE = $1 * 137 \times 10^3$ Btu/gal $* 8.48 \times 10^{-5}$ lb/10^6 Btu $* 1.6694 \times 10^3$ gal/yr

= 0.0194 lb/yr Naphthalene

AQUIS Printout: AAUE = 0.019 lb/yr Naphthalene

FIGURE 3.4-2. CONTINUED

5

COMPUTERIZED CHECKS

QUICK REVIEW

Definition:	Electronic methods of checking or verifying data or emissions; they may be a built-in function of an emissions database, model, or spreadsheet, or they may be stand-alone programs.
Objective:	Ensure the accuracy or correctness of a value.
Optimal usage:	Generally used for QC at the point where data are being entered into a computer software program for further processing and/or after emissions have been calculated. Frequency and timing of use depend mostly on the specific technology.
Minimum expertise required:	Low to moderate, depending on the specific tool/method.
Advantages:	(1) Built-in checks can be done with little additional effort and the need for more laborious manual reviews may be eliminated, (2) they allow efficient checking of large amounts of data, and (3) certain software features prevent or minimize some types of errors.
Limitations:	(1) Requires some level of human decision-making (such as determining whether a variable that is outside a range is really an error), (2) some programs--particularly stand-alone programs--require additional training or expertise to use properly, (3) all require a computer, (4) too much reliance may be placed on the computer's ability to detect errors, resulting in too little QA/QC by humans, and (5) cannot catch erroneous values that pass range/limits checks.

5.1 OVERVIEW OF METHOD

Automated checks cover a wide array of computer-based QA/QC functions. They include: (1) common features found in most database programs or models that ensure against entering characters where numbers are expected, (2) range checks that give an expected minimum and maximum for a specific variable, and (3) look-up tables that define permissible entries, and The user is given a message or printed report to document the potential problem. Some computer programs provide users with visual written QA/QC tools. Spreadsheet audit functions, for example, can map cell references and formulas visually in report format. Other computer programs are designed to display data visually through maps, charts, or graphics. These features vary in their implementation between computer programs; it is important that the user understand how they work and then use these features correctly.

Unlike the methods described in previous sections of this chapter, the inventory preparers may have very little choice in selecting automated checks because the emissions estimation system may already have been chosen (or may be outside their control). However, the automated checks described in this section do not provide any new functions; they are automated, efficient ways to screen, summarize, and/or present data for "Peer Review" (Section 3) or "Independent Audits" (Section 8). This section describes some of the general QA/QC functions used in emissions estimation software, such as:

- Features of spreadsheets that can be used to facilitate QA/QC; and

- Some stand-alone software programs that can be used in QA/QC tools.

The computer-literate inventory preparer is encouraged to develop his/her own automated QA/QC programs using the ideas presented here.

Automated QA/QC functions can be used to facilitate peer review or, in some cases, replace manual reality checks. Because large amounts of data can be processed very quickly, these computer-based methods can significantly reduce the amount of time required both to develop and quality assure an inventory. In addition, some of the data entry features used in computer-based estimation software that were designed primarily to simplify data entry also help reduce the number of potential errors. By reducing the amount of information that has to be entered manually, the number of typographical errors is reduced. Furthermore, some programs select the correct emission factor (or other defaults needed to estimate emissions) based on one or more parameters provided by the user. Although they may not eliminate errors, these automated procedures can help reduce the use of incorrect data.

It is important to note that these reports do not actually perform QA functions. Reports that are designed to highlight outliers or suspect data do just that--highlight *suspect* data. Similarly, reports that display information only display information as requested. Human

reasoning and judgment must still be applied when reviewing the reports and evaluating them for errors. The preferred method for emissions estimation and performance of many types of QA/QC checks is to use emissions-estimation software with built-in QA/QC functions and data entry procedures that minimize errors. If that is not feasible, the second-best method is to develop standardized spreadsheets or databases using standard software packages, building in as many QA features as possible. Most popular spreadsheet and database packages support the use of look-up tables and provide auditing tools that can be used for QA/QC. Portions of the spreadsheet or database file can be locked or protected to prevent inadvertent changes.

Because the programmer is often not the end user, it is highly recommended that the end user be involved in developing the program and its output features. Involving the user will help maximize the usefulness of the program and make it more user friendly.

Emissions-estimation software or spreadsheet/database programs can be supplemented using stand-alone programs to check or review the data. Some programs provide range checks on data, generating reports that flag potential problems. Emissions estimates can be further verified by using data visualization programs. These software programs are capable of transferring emissions data from spreadsheet/database format to visual tools such as points on a map, charts, and tables.

Table 3.5-1 summarizes the methods and functions described in this section. Preferred and alternative methods were not defined for this group of tools because the technology available to different agencies varies.

As valuable as these automated tools are, they do have some limitations, such as creating a false sense of confidence in the data. It is usually necessary for a reviewer to make a judgment about the data quality by reviewing the computer-generated reports or error messages and deciding which potential errors need to be corrected. Also, even if the value for a particular parameter is within a reasonable range, it can still be wrong. Therefore, these automated tools are not a substitute for peer reviews or audits; rather, they should be used to facilitate other QA/QC activities.

Most emissions-estimation software offers built-in functions designed to prevent the introduction of faulty data into the emissions calculation. Functions such as range and data-type checks are QA functions that flag potential errors. Other features are indirect forms of QA in that they reduce the amount of data that must be entered or limit the options. These features include look-up tables and pull-down menus where the user must choose from a limited but inclusive list of options. Although not necessarily meant as a QA tool, these features can help minimize several types of data-entry errors.

TABLE 3.5-1

SUMMARY OF COMMON AUTOMATED CHECKS

Type of Automated Check	Description	Examples	Strengths/Limitations
Variable type check	Alerts user if wrong data type or inappropriate value is entered.	Numeric value is expected, character string entered: a warning is issued immediately or field is flagged in subsequent report.	Reduces errors early in process, especially if warning issued interactively and/or if incorrect data entry prohibited. Report in which error is flagged is easily ignored.
Range (value) checks	Checks value entered to determine if it is within an expected or acceptable range.	Range of stack heights is used to flag a stack height that is too high or low.	Flags suspicious data for further review. Does not eliminate possibility that wrong value entered is within range, or that value outside range could still be correct.
Look-up table	Uses a parameter (such as user-supplied input variable) to select other appropriate parameters from a table.	User enters a source category code (SCC) and program supplies appropriate emission factor.	Eliminates some types of data entry errors; assures data consistency. If wrong value added (i.e., incorrect SCC), all dependent values will also be wrong.
Pull-down menu, pop-up window	Presents selection of possible values for a particular field.	List of possible fuel types is presented to user when entering data to calculate boiler emissions.	Eliminates transcription errors, reduces chance of using wrong value due to user not understanding what is wanted. Does not eliminate possibility that wrong choice will be made by user.
Completeness/ Consistency checks	These two terms are often used to describe similar operations; include a wide array of checks and/or comparisons.	Checks verify that some specified amount of data for certain fields has been entered; or, if a certain field has data, verifies that other required fields also have data. Assure that units, equipment types, IDs, and other parameters are consistent.	Completeness is often difficult to quantify; in practice, a minimum expected value is used to determine completeness. Does not assure that data are correct. Impossible to completely automate these types of checks, some expert judgment usually required. If too much consistency automated into process, inflexibility may result.

5.1.1 RANGE AND CHARACTER CHECKS

Data-type checks prohibit the user from entering text strings when numerical values are expected and vice versa. In most cases, data-type and range checks are no more than an automated reality check. Range checks provide an indication that the value is (or is not) within an expected range. However, these checks do not necessarily ensure that the value is correct. Also, range checks may warn the user of a potential problem, but do not usually prevent entry of incorrect data.

Numerical range checks generally fall into one of two categories: (1) the upper and/or lower limit is specified, or (2) the statistical mean or median is used as a point of reference. In the first case, as long as the input value falls within (or above or below) the limit, no error is flagged. Setting this limit is difficult; assuming an upper bound is used, if it is set too high, no potential errors are flagged. If set too low, too many data points are flagged. The use of statistically derived reference values raises similar questions (see Section 7, "Statistical Checks," of this chapter).

A common frustration that many inventory preparers have with automated QA checks that use an average (or default) value as a reference point is that correct, site-specific data are often either higher or lower than a statistical average or default. This flagging of correct but atypical values should not be viewed as a problem with the system; rather, it provides the opportunity to review and explain the data. The *perceived* quality of the inventory to the user or reviewer is increased by this sort of analysis, even though the *real* quality is unchanged. In other words, confidence in the emission estimates has increased.

5.1.2 LOOK-UP TABLES

Look-up tables are another feature of many computer programs. They help ensure data quality by restricting the number of choices a user has to make. A look-up table uses one variable (entered by the user) to look up the correct value for another variable.

For example, some computerized emissions calculation programs supply the correct emission factor by matching it to a source category code (SCC). One approach is to retrieve the correct emission factor based on an SCC entered by the user. Although this ensures a correct match between the code and the factor, if the user enters the incorrect code, the emissions will be calculated with the wrong number. Therefore, look-up tables are not always foolproof.

Other systems minimize this type of error by building more safeguards into the system. The AQUIS used by the U.S. Air Force, Air Combat Command, has separate modules for each source type. To calculate boiler emissions, for example, the user enters the boiler characteristics, fuel use, and fuel type in the "External Combustion" module. The program

uses this information to select the correct emission factor. The possibility of error still exists because incorrect boiler data could result in the selection of an incorrect emission factor; however, it is less likely to occur than when the additional step of supplying the correct SCC is required.

Still other systems allow the user to set up the relationships in the look-up table. This approach is used in some commercial emissions database software. Access to these tables is limited to a system administrator who can assign codes, emission factors, and specify other interrelationships between data to be entered in the system. Usually these software packages allow the user to enter alternative emission factors, conversion factors, or constants. The inventory developer using this type of software should take advantage of these features to build in QA/QC features.

5.1.3 PULL-DOWN MENUS AND POP-UP WINDOWS

Another error-limiting feature is the pull-down menu or pop-up window. This feature is activated when the user selects a field to enter data. The menu/window will appear and offer a limited set of allowable entries.

5.2 INTERNAL CHECKS AND REPORTS: CEIDARS, RAPIDS, STANDARDIZED SPREADSHEETS

After the data for performing the emissions calculations have been entered, many programs have internal QC programs designed to highlight suspect information for further evaluation. These programs are a form of "reality check," but are capable of processing larger volumes of data than a human reviewer, automatically flagging input/output that falls outside the expected parameters. However, the flagged data must be reviewed by a human to determine whether an error has really occurred. Software packages, such as the Regional Air Pollutant Inventory Development System (RAPIDS) and California Emissions Inventory Database Acquisition Retrieval System (CEIDARS) contain built-in checks and reports designed to evaluate data and present potential errors or highlight important information. Other software packages may allow the user to design a QC report that prints key variables. Depending on the flexibility of the software, the user may be able to design QA reports that perform some of the same functions as described below for CEIDARS and RAPIDS.

5.2.1 CEIDARS

The California Air Resources Board (ARB) uses an Oracle®-based relational database system to compile and maintain toxic and criteria air pollutant inventories. This system, CEIDARS, also provides many built-in QA functions that are used by the state agency to review data entered at the district level (California is divided into multiple air districts each with its own staff responsible for developing inventories and performing other functions). These data

have presumably undergone QA/QC checks prior to submittal to the district, and reviewed at the district level prior to entry into CEIDARS (see Chapter 2 of this volume, *Planning and Documentation* for a description of the ARB's QA procedures designed to use these reports).

Eleven different QA reports are provided in CEIDARS; the differences between them are defined partly by the QA features and partly by the category type or level (e.g., area, point, stack).

To ensure the integrity and completeness of the criteria pollutant data, the CEIDARS QA reports are designed to help identify errors, inconsistencies, or omissions in the criteria pollutant inventory data input to the database. The QA reports verify that all critical data fields for each facility are entered into the database, and that various data consistency and range-checking criteria are met. The QA reports are not for general data (emissions) reporting.

Some CEIDARS reports perform integrity checks on data entered by the user (QAFACC, QASTKC, QACEVE, QAPROC). Other reports check key field data (QAKEYS), or the consistency of emissions data with reported process rates and emission factors (QAKEMS). QA reports also perform validity and range checking of various data including stack (QASTACK) and temporal (QATEMP) information.

Completeness Checks

Four different reports perform some completeness checks at the facility, stack, device, and process levels. The facility-level report verifies that at least one emissions record is reported for each facility. If a record is flagged, the reason for the lack of emissions is investigated. If emissions were reported but not entered, the district must resolve the error. However, if no facility emissions were reported (by the facility operator), the record may either be dropped or retained (for tracking). Similar reports flag stacks, devices, and processes that do not have any reported emissions. As with the facility QA report, the reviewer must determine if the omission is truly an error.

Consistency/Validity Checks

Several QA reports are designed to flag inconsistent, invalid, or missing data. One report checks to ensure that key data are present and consistent. For example, if a device has not been defined for a process, the error message "DEVICE NUMBER IS MISSING OR INCONSISTENT" is given. The items checked include county identification (ID) and name; device ID; facility ID, name, and Standard Industrial Classification (SIC) code; pollutant ID and name; process ID, SCC, and SIC codes; and stack ID.

A similar type of data check is performed on process and emissions data to verify that they are valid and consistent. For example, an error is flagged if an invalid emissions estimation code is used. If emissions are reported when the process rate is zero, an error is flagged. The validity of the reported emissions is checked by comparing it to a calculated value (i.e., process rate times an emission factor); if the two values are not within 10 percent of each other, the record is flagged. The items checked include emissions, fraction particulate matter (PM), district-specified reactive organic gas (ROG), PM less than or equal to 10 μm (PM_{10}), fraction ROG, process rate, and sulfur content.

Stack data validity is checked and verified to be within expected ranges by another set of QA checks. For example, if the stack temperature is less than 50°F or greater than 2000°F, an error is flagged. If the flow rate reported for the stack does not equal a computed theoretical flow rate (± 10 percent), an error is flagged. Stack parameters checked include gas flow, gas temperature, gas velocity, stack diameter, stack height, and universal transverse mercator (UTM) coordinates.

Other reports verify the spatial and temporal data, device and process data, and control device data. The spatial and temporal parameters checked include days per week/weekly operating cycle, hours per day/daily operating cycle, and operating weeks per year. The device and process data reported are device ID, equipment size, equipment type code, equipment size unit code, maximum design rate, process rate, and process description.

5.2.2 RAPIDS

RAPIDS is a database management system developed specifically for compiling and maintaining state toxic emissions data into a central regional repository. States using this system have available many QA/QC functions in RAPIDS that should be used prior to submitting their toxic emissions data and estimates into the regional repository. The objective of these QC checks is to ensure that the regional database of emissions data and estimates is as complete as practicable and is properly QA checked. Below is a list of the QC checks performed by RAPIDS:

- *Data integrity checks*: Ensure that no invalid relationships among data elements exist (e.g., no process without a device, device without a facility, material activity without a material).

- *Field-specific checks*: Ensure that obviously invalid data are not entered into the database [e.g., SIC code, SCC/Area and Mobile Source Subsystem (AMS) Codes, speciation factor (>0.0 to <1.0), data relationships, etc.].

- *Record-specific checks*: Identify a valid relationship between two values in different fields in the same record (e.g., installation date is earlier than the

> dismantling date of a facility or device, start date/time in an activity record is
> earlier than the current date).

- *Cross-entity checks*: Identify invalid relationships between data in two
  different entities (i.e., data elements).

- *Completeness checks*: Refer to the extent to which all sources/devices/
  processes and emittants are accounted for in the inventory database.

- *Consistency and reasonableness checks*: Consistency refers to the extent that
  emissions data and estimates do not significantly vary among similar
  occurrences of the same area, source, device, process, stream, etc.
  Reasonableness refers to the extent that emissions data meet certain
  expectations based on experience.

The last two types of QC checks identify *possible* errors and require manual investigation to
determine if an error really exists and how to correct it. Completeness or consistency and
reasonableness QC checks do not lend themselves to inclusion as fully automated checks;
rather, they require the user to generate reports or other outputs from general purpose
software to identify possible errors in the data.

5.2.3 STANDARDIZED SPREADSHEETS/DATABASES

If emissions are to be calculated using spreadsheet or database software, many of the QA/QC
features available in emissions-estimation software can be built into standardized
spreadsheets or simple database programs. The additional effort required should pay off if
the inventory is large, if it may be repeated or updated periodically, or if data entry may be
performed by more than one person.

Area Source Inventory Spreadsheet Example

Standardized spreadsheets were developed and used to prepare an area source Level 4
inventory of air toxics in the Puget Sound region. The inventory preparation plan specifies
the methods, factors, and speciation profiles used on the spreadsheet. All inventory
personnel had a copy of the plan.

Figure 3.5-1 shows the spreadsheet developed for calculating graphics arts hazardous air
pollutants (HAPs). It is one of many spreadsheets used to calculate area source HAP
emissions for an urban area. The basic spreadsheets were developed by one person; the cells
for activity data and any other user-defined parameters were left blank (shown in italics in
Figure 3.5-1). The source-specific VOC emission factors and HAP speciation profiles were
included in the spreadsheet. The user (i.e., the person calculating emissions for a category)

FIGURE 3.5-1. EXAMPLE OF STANDARDIZED SPREADSHEET FOR AN AREA SOURCE

Created by: M. Adams	Data entry by:	QC by:
Date: 11/03/94	Date:	Date:
Purpose: Calculate HAPs from graphic arts in Ozoneville using EPA VOC per capita methods and speciation profiles.		
SOURCE CATEGORY:	Graphic Arts	
AMS Code	2425000000	

County		County A	County B	County C
Zone 1 population		1,364,576	510,524	368,416
Zone 2 population		142,743	75,679	97,226
Total population, Zones 1 & 2		1,507,319	586,203	465,642
VOC emission factor, lb/capita		1.3	1.3	1.3
Adjustments (if none, enter 1)		1	1	1
VOC emissions (pounds)		1,959,515	762,064	605,335

HAP NAME	HAP CODE	HAP Emissions (pounds/year)		
Xylene	1	189,955	73,874	58,681
Toluene	2	229,812	89,375	70,994
Glycol ethers	3	346,834	134,885	107,144
Methyl ethyl ketone	4	70,543	27,434	21,792
Ethylbenzene	5	12,169	4,732	3,759
Ethylene glycol butyl ether	6	109,733	42,676	33,899
Diethylene glycol butyl ether	7	92,097	35,817	28,451
Other diethylene glycol ethers	8	74,462	28,958	23,003
Propylene glycol methyl ether acetate	9	21,555	8,383	6,659
Ethylene glycol ethyl ether acetate	10	13,717	5,334	4,237
Other glycol ethers and esters	11	35,271	13,717	10,896
Glycols (unsubstituted)	12	35,271	13,717	10,896
County Total		1,231,418	478,904	380,410

FIGURE 3.5-1. CONTINUED

SPECIATION PROFILES		WEIGHT PERCENT OF VOC VAPORS
HAP	HAP CODE	Graphic Arts
Xylene	1	9.69%
Toluene	2	11.73%
Glycol ethers	3	17.70%
Methyl ethyl ketone	4	3.60%
Ethylbenzene	5	0.62%
Ethylene glycol butyl ether	6	5.60%
Diethylene glycol butyl ether	7	4.70%
Other diethylene glycol ethers	8	3.80%
Propylene glycol methyl ether acetate	9	1.10%
Ethylene glycol ethyl ether acetate	10	0.70%
Other glycol ethers and esters	11	1.80%
Glycols (unsubstituted)	12	1.80%

entered the needed data and emissions were automatically calculated. A look-up function uses the HAP code to find the weight percentage (shown in the last table in the spreadsheet) used to estimate the HAPs value.

If spreadsheets must be used for inventory estimates, developing standardized spreadsheets has several advantages for QC. The spreadsheets (without activity data) can undergo QA/QC checks before emissions are calculated and all cells except those needed for data input can be locked (or protected). This will ensure that changes to the data are not made inadvertently. Final QA of the estimates is simplified because only activity data (and any other user-supplied data) need to be reviewed. This method may help eliminate a "QA bottleneck" at the end of the project by dividing the review into several segments.

Another advantage of this system is that the emissions were easily imported into a database for summation and reporting. The format of the spreadsheets was designed so that the emissions were always in a block and in the same pollutant (rows) and county (columns) order. This makes import of the results into a summary spreadsheet or a database program relatively simple. Also, it minimizes the chance of errors in data transfer and compilation.

Point Source Inventory Spreadsheet Example

The North Carolina Department of Environment, Health, and Natural Resources (NC DEHNR) has developed standardized spreadsheets for some types of emissions sources that are currently permitted. These spreadsheets are available to facilities that are preparing permit applications or annual emissions inventories (for fee assessments). An example of one of these spreadsheets is shown in Figure 3.5-2. This spreadsheet uses cell protection so that the user cannot change emission factors or other crucial data. Look-up functions are used to select the correct emission factor and to calculate emissions. If the user wishes to calculate potential emissions, the "ACTUAL NG BURNED" box is left blank; the spreadsheet then uses the data shown under "FOR POTENTIAL" to calculate potential emissions. An example is shown in Figure 3.5-3.

This spreadsheet illustrates some other good QA features. The sources of the factors and the assumptions used are shown in the "NOTES" near the bottom of the page. This spreadsheet does not show a version number (or date created/revised), but some other DEHNR spreadsheets do. Some sort of document control system that uses identifiers, dates, and/or authorship to track different versions of spreadsheets is a good idea, especially when they are distributed widely.

5.2.4 SPREADSHEET AUDITING FUNCTIONS

For emissions that are calculated by spreadsheet applications, audit functions built into most spreadsheet software provide the user and checker with a helpful tool for verifying formula

Natural Gas Combustion: Criteria and Toxic Air Pollutant Emissions | Central Office Version

NAME OF FACILITY: No Name Co. | APP
CITY: Rocky Mount | Review Engineer   R. Person
COUNTY: Nash

Boiler Input Data

| BOILER TYPE > | 2 |

1 - LARGE BOILER > 100 mmBtu/hr
2 - SMALL BOILER 10 - 100 mmBtu/hr
3 - COMMERCIAL < 10 mmBtu/hr

ACTUAL NG BURNED : 35.00 mm cu. ft/yr

.0503 PM Allowable
FOR POTENTIAL : | 0.47 lb/mmBtu
ENTER BOILER SIZE : 25 mmBtu/hr | 11.9 lb/hr @ max. input
HOURS OF OPERATION : 8,760 hr/yr | .0516 SO2 Allowable
ENTER % CONTROL EFF. : 0.00 % | 58 lb/hr @ max. input

ACTUAL CRITERIA EMISSIONS

Pollutant	Factor (lb poll./1E6 cu. ft burned)	(lb/yr)	(lb/hr)	(tpy)
TSP	13.7	480	0.05	0.24
PM-10	13.7	480	0.05	0.24
SOx	0.6	21	0.00	0.01
NOx	140.0	4,900	0.56	2.45
VOCs	2.8	97	0.01	0.05
CO	35.0	1,225	0.14	0.61

ACTUAL TOXIC EMISSIONS

Pollutant	Factor (lb poll./1E12 Btu)	(lb/yr)	(lb/hr)	(tpy)
FORMALDEHYDE	220.3	7.9	9.07E-04	0.004

Potential NG usage : 214 mm cu. ft/yr   24,379 cu. ft/hr
Heating value : 1,030 Btu/cu. ft

NOTES:
FACTOR #1 - AP-42, SUPPLEMENT F (7/93), SEC 1.3
FACTOR #2 - EPA 450/2-90-011

ASSUMPTIONS:
- TSP, PM10, AND POM ARE AFFECTED BY CONTROL
- HEAT CONTENT OF NG 1030 Btu/cu.ft
VOCS = TOC*(1-%METHANE)

Disclaimer
"This spreadsheet is for your use only and should be used with caution. DEHNR does not guarantee the accuracy of the information contained. This is a draft spreadsheet and is continually revised and updated. It is your responsibility to be aware of the most current information available. DEHNR is not responsible for errors or omissions that may be contained herein."

FIGURE 3.5-2. EXAMPLE OF STANDARDIZED SPREADSHEET FOR POINT SOURCE ACTUAL EMISSIONS

Natural Gas Combustion: Criteria and Toxic Air Pollutant Emissions   Central Office Version

NAME OF FACILITY: No Name Co.   APP

CITY: Rocky Mount   Review Engineer   R. Person

COUNTY: Nash

Boiler Input Data

BOILER TYPE >	2

1 - LARGE BOILER > 100 mmBtu/hr

2 - SMALL BOILER 10 - 100 mmBtu/hr

3 - COMMERCIAL < 10 mmBtu/hr

ACTUAL NG BURNED :   mm cu. ft/yr

.0503 PM Allowable

FOR POTENTIAL :   0.47   lb/mmBtu

ENTER BOILER SIZE :   25   mmBtu/hr   11.9   lb/hr @ max. input

HOURS OF OPERATION :   8,760   hr/yr   .0516 SO2 Allowable

ENTER % CONTROL EFF.   0.00   %   58   lb/hr @ max. input
:

POTENTIAL CRITERIA EMISSIONS

Pollutant	Factor (lb poll./1E6 cu. ft burned)	Emission Rates (lb/yr)	(lb/hr)	(tpy)
TSP	13.7	2,926	0.33	1.46
PM-10	13.7	2,926	0.33	1.46
SOx	0.6	128	0.01	0.06
NOx	140.0	29,898	3.41	14.95
VOCs	2.8	595	0.07	0.30
CO	35.0	7,474	0.85	3.74

POTENTIAL TOXIC EMISSIONS

Pollutant	Factor (lb poll./1E12 Btu)	Emission Rates (lb/yr)	(lb/hr)	(tpy)
FORMALDEHYDE	220.3	48.5	5.53E-03	0.024

Potential NG usage :   214   mm cu. ft/yr   24,379   cu. ft/hr

Heating value :   1,030   Btu/cu. ft

NOTES: ASSUMPTIONS:
  FACTOR #1 - AP-42, SUPPLEMENT F (7/93), SEC 1.3   - TSP, PM10, AND POM ARE AFFECTED BY
  FACTOR #2 - EPA 450/2-90-011   CONTROL
                                                   - HEAT CONTENT OF NG 1030 Btu/cu.ft
                                                     VOCS = TOC*(1-%METHANE)

Disclaimer

"This spreadsheet is for your use only and should be used with caution. DEHNR does not guarantee the accuracy of the information contained. This is a draft spreadsheet and is continually revised and updated. It is your responsibility to be aware of the most current information available. DEHNR is not responsible for errors or omissions that may be contained herein."

FIGURE 3.5-3. POINT SOURCE SPREADSHEET TOGGLED TO PRODUCE POTENTIAL EMISSIONS

calculations and cell references. Although many spreadsheets have their own specific auditing functions, some of the more common audit options include cell dependency, cell precedence, and error identification. Although these are three different functions, they all share one important characteristic: they help the user identify which cells are referenced in spreadsheet formulas.

Figure 3.5-4 is an example of Excel tracing cell precedents. By highlighting a cell with a formula in it and selecting the *tools/audit/cell precedents* function, Excel displays on-screen arrows that point to the cells used in the calculation, allowing an auditor to quickly and easily verify formulas and calculations. The Lotus audit function operates in a similar fashion by highlighting all cells used in formula calculations.

Both Excel and Lotus provide the user with the ability to generate a description of cells involved in a calculation. Figure 3.5-5 illustrates the "report" generated by Lotus when a cell is selected and the *audit/trace dependents* function is activated.

5.3 STAND-ALONE PROGRAMS

Additional QA/QC functions are available through the use of stand-alone programs developed primarily for this purpose. These include programs with the same types of features as those described above, as well as graphical and mapping systems that can be used to perform visual auditing of data.

5.3.1 EIQA

Emission Inventory Quality Assurance (EIQA) is a software program specifically designed to provide QA/QC capabilities. EIQA provides an automated means of performing QA edit checks on critical data elements in the emissions inventories submitted by the states to the EPA's Aerometric Information Retrieval System (AIRS); it has also been adapted for use on non-AIRS data. The EIQA program is available for general use on EPA's mainframe computer; however, user support is not provided by the EPA. Reports can be generated that examine the data for point, area, and mobile sources, and MOBILE model input data. By providing the user with an automated checking and reporting system, the net result should be significantly improved quality of the emissions inventory data stored in AIRS. A sample of QA reports generated by EIQA for point, area, and mobile source data are listed below.

Point source data QA reports include:

- Range Checks [compares inputs on an SCC-basis to a range of expected values from 1985 National Acid Precipitation Assessment Program (NAPAP) inventory];

Table 1 Component Count for Equipment Leak Emission Sources

Item Utilized Approx 100%	Pump Seals	Valves	Safety Release Valves	Flanges	Open-Ended Lines
Train Offloaders	0	11	0	176	0
Truck Fuel Stand	0	3	1	14	2
Tanks	0	4	0	19	0
Pumphouse	5	23	7	55	5
Total	5	41	8	264	7

Table 2 Fugitive Emissions from POL Equipment Components

Component	Total Items	Emission Factor (kg HC/hr-unit)	Yearly Emissions (tons VOC/yr)
Pump Seals	5	0.000423	0.02
Valves	41	0.000068	0.03
Safety Release Valves	8	0.000114	0.01
Flanges	264	0.0001045	0.27
Open-Ended Lines	7	0.002954	0.20
Total Fugitive Emissions (tons VOC/yr)			0.52
Total Fugitive Emissions (lbs VOC/yr)			1044.42

Table 3 HAP Speciation Data

Regulated Pollutant	Percent by Weight for JP-4
Benzene	0.5
Biphenyl	...
Hexane, n-	2.21
Naphthalene	0.5
Toluene	1.33
Xylene, M-	0.96
Xylene, o-	1.01
Xylene, p-	0.35

Table 4 Actual Emissions from POL Equipment Leaks

Regulated Pollutant	Emissions (lb/yr)
Benzene	5.2
Biphenyl	0
Hexane, n-	23.1
Naphthalene	5.2
Toluene	13.9
Xylene, M-	10.0
Xylene, o-	10.5
Xylene, p-	3.7

FIGURE 3.5-4. EXAMPLE OF VISUAL TRACING OF CELLS USING A SPREADSHEET AUDIT FUNCTION

Table 1 Component Count for Equipment Leak Emission Sources

Item Utilized Approx 100%	Pump Seals	Valves	Safety Release Valves	Flanges	Open-Ended Lines
Train Offloaders	0	11	0	176	0
Truck Fuel Stand	0	3	1	14	2
Tanks	0	4	0	19	0
Pumphouse	5	23	7	55	5
Total	5	41	8	264	7

Table 2 Fugitive Emissions from POL Equipment Components

Component	Total Items	Emission Factor (kg HC/hr-unit)	Yearly Emissions (tons VOC/yr)
Pump Seals	5	0.000423	0.02
Valves	41	0.000068	0.03
Safety Release Valves	8	0.000114	0.01
Flanges	264	0.0001045	0.27
Open-Ended Lines	7	0.002954	0.20
Total Fugitive Emissions (tons VOC/yr)			0.52
Total Fugitive Emissions (lbs VOC/yr)			1044.42

Table 3 HAP Speciation Data

Regulated Pollutant	Percent by Weight for JP-4
Benzene	0.5
Biphenyl	---
Hexane, n-	2.21
Naphthalene	0.5
Toluene	1.33
Xylene, M-	0.96
Xylene, o-	1.01
Xylene, p-	0.35

FIGURE 3.5-5. EXAMPLE OF CELL FORMULAS LISTING USING A SPREADSHEET AUDIT FUNCTION

Table 4 Actual Emissions from POL Equipment Leaks

Regulated Pollutant	Emissions (lb/yr)
Benzene	5.2
Biphenyl	0
Hexane, n-	23.1
Naphthalene	5.2
Toluene	13.9
Xylene, M-	10.0
Xylene, o-	10.5
Xylene, p-	3.7

Precedents of Cell A:D38
Current file
A:C38: 'Benzene
A:F22: 'Benzene
A:F23: 'Biphenyl
A:F24: 'Hexane, n-
A:F25: 'Naphthalene
A:F26: 'Toluene
A:F27: 'Xylene, M-
A:F28: 'Xylene, o-
A:F29: 'Xylene, p-
A:G22: 0.5
A:G23: '---
A:G24: 2.21
A:G25: 0.5
A:G26: 1.33
A:G27: 0.96
A:G28: 1.01

A:G29: 0.35
A:D28: +D27*2000
A:D27: @SUM(D22..D26)
A:D22: +B22*C22*8760/907.
A:D23: +B23*C23*8760/907.
A:D24: +B24*C24*8760/907.
A:D25: +B25*C25*8760/907.
A:D26: +B26*C26*8760/907.
A:B22: +B11
A:C22: 0.000423
A:B23: +C11
A:C23: 6.8E-05
A:B24: +D11
A:C24: 0.000114
A:B25: +E11
A:C25: 0.0001045
A:B26: +F11
A:C26: 0.002954

A:B11: @SUM(B7..B10)   A:E8: 14
A:C11: @SUM(C7..C10)   A:E9: 19
A:D11: @SUM(D7..D10   A:E10: 55
A:E11: @SUM(E7..E10)   A:F7: 0
A:F11: @SUM(F7..F10)   A:F8: 2
A:B7: 0   A:F9: 0
A:B8: 0   A:F10: 5
A:B9: 0
A:B10: 5
A:C7: 11
A:C8: 3
A:C9: 4
A:C10: 23
A:D7: 0
A:D8: 1
A:D9: 0
A:D10: 7
A:E7: 176

FIGURE 3.5-5. CONTINUED

- Consistency Checks (ensures that certain data elements are correct);

- Report Emission by Miscellaneous SCC Summary [shows emission totals by the SCC that are "miscellaneous" source types of VOCs, NO_x, and carbon monoxide (CO)];

- Report Emission by Method Code Summary (reflects the percentage of the total emissions for a pollutant that was obtained by a certain method);

- Report Emission by Source Magnitude Summary (indicates the magnitude of source in the inventory region);

- Report Source Category Completeness Summary (highlights where "expected" data are missing);

- Report Rule Effectiveness Category Summary (reports on the existence of rule-effectiveness estimates in the AIRS Facility Subsystem (AFS) for selected SIC/SCC combinations that are expected to have rule-effectiveness estimates); and

- Report Plants Exceeding 500 Tons Per Year (tpy) Summary [indicates the plants exceeding 500 tpy per pollutant listed (classified by pollutant)].

Figure 3.5-6 shows an example of a source category completeness summary.

Area source data QA reports include:

- Activity Level Unit Range Check Exceptions (the AMS database includes acceptable SCC-specific activity levels; these data are used to check the reported activity level units in the inventory);

- Fuel Loading Factor Range Check Exceptions (the minimum and maximum fuel loading factors, as found in the EPA document, *Compilation of Air Pollutant Emission Factors Volume I: Stationary Point and Area Sources*, commonly referred to as AP-42, are used to identify the inventory's outliers);

- Base Year Factor Range Check Exceptions (reports records in which the base year does not equal the designated year, 1990);

- Annual Emissions Range Check Exceptions (the EPA document, *Quality Review Guidelines for 1990 Base Year Emission Inventories*, defines per capita

EMISSION INVENTORY QUALITY ASSURANCE SYSTEM
POINT SOURCES
SOURCE CATEGORY COMPLETENESS SUMMARY REPORT F

BASE YEAR: 1990 SIP PROGRAM: OZONE STATUS AREA CODE: N0200 DATE REPORT GENERATED: 07JUL94

DEFINITION OF REPORT F:
These source categories and ranges are expected in most
nonattainment areas as listed in EPA's Quality Review Guidelines.
An "N" in the "PRESENT" column may indicate and incomplete inventory.

PRIORITY RANKING SCHEME:
1 = High Priority   - Resolution/Determination Required
2 = Warning/Advisory   - No Formal Action Required
3 = Informative   - See Text for Further Description

EMISSION INVENTORY QUALITY ASSURANCE SYSTEM
POINT SOURCES
SOURCE CATEGORY COMPLETENESS SUMMARY REPORT F

BASE YEAR: 1990 SIP PROGRAM: OZONE STATUS AREA CODE: N0200 DATE REPORT GENERATED: 07JUL94
Priority 1: High Priority

Exception Resolution	SCC	Source Category Name	Emission Magnitude Range	Pollutant	Present
____	4-05-xxx-xx	Graphic Arts	10-25 tpy	VOC	N
____	1-03-xxx-xx	Commercial Boilers	10-25 tpy	NO_x	N
____	1-03-xxx-xx	Commercial Boilers	10-25 tpy	CO	Y
____	4-04-xxx-xx	Petroleum Storage	>25 tpy	VOC	N
____	4-06-xxx-xx	Petroleum Market & Transport	>25 tpy	VOC	N
____	3-xx-xxx-xx	Industrial Processes	all ranges	all	Y
____	1-02-xxx-xx	Industrial Boilers	all ranges	NO_x	Y
____	1-02-xxx-xx	Industrial Boilers	all ranges	CO	Y
____	1-01-xxx-xx	Utility Boilers	all ranges	NO_x	N
____	1-01-xxx-xx	Utility Boilers	all ranges	CO	N

FIGURE 3.5-6. EIQA POINT SOURCES COMPLETENESS REPORT

range checks for area source emission categories; the program uses these ranges to identify SCCs that are apparently under- or over-reported);

•   SIP Rule in Place Consistency Check (identifies area sources that may be covered under SIP rules);

•   Pollutant Consistency Check Exceptions (checks for pollutants not reported for certain SCC codes);

•   Gasoline Consumption Consistency Check Exceptions [compares gasoline consumption to population estimates and expected state-level Department of Energy (DOE) gasoline consumption estimates];

•   Population Consistency Check Exceptions (highlights large population changes);

•   Emission Factor Units Consistency Check Exceptions (highlights where factor units are not what were expected);

•   SCC Consistency Check Exceptions (highlights potentially missing SCCs); and

•   Annual Emission Consistency Check Exceptions (highlights large changes in emissions from prior levels).

An example of an area source report (SIP Rule in Place Consistency Check) is shown in Figure 3.5-7.

Mobile source data QA reports include:

•   Range Check Exception Report (expected values for specified vehicles);

•   Period Consistency Check Exception Report (checks are designed to ensure internal consistency of source data);

•   VMT Consistency Check Exception Report (checks reported VMTs against expected values);

•   Data Item Completeness Exception Report (checks for amount of road type, expected pollutant levels, etc.);

•   SCC, VMT, and Emissions Summary Report (assists user in performing manual examination of inventory data);

EMISSION INVENTORY QUALITY ASSURANCE SYSTEM
AREA SOURCES
SIP RULE IN PLACE CONSISTENCY CHECK EXCEPTION REPORT E

BASE YEAR: 1990 FILENAME: AREADAT DATE REPORT GENERATED: 07JUL94

DEFINITION OF REPORT E:
Area sources may be covered under SIP rules in some areas.
Check that this report is consistent with local rules.

PRIORITY RANKING SCHEME:
1 = High Priority   - Resolution/Determination Required
2 = Warning/Advisory - No Formal Action Required
3 = Informative   - See Text for Further Description

EMISSION INVENTORY QUALITY ASSURANCE SYSTEM
AREA SOURCES
SIP RULE IN PLACE CONSISTENCY CHECK EXCEPTION REPORT E

BASE YEAR: 1990 FILENAME: AREADAT DATE REPORT GENERATED: 07JUL94
Priority 1: High Priority

Exception Resolution	ST CNTY CITY ZN	SCC	SCC Description	Pollutant	SIP Rule in Place Reported	SIP Rule in Place Expected	Rule Effective- ness	Rule Penetra- tion
_____	18 005	24-15-300-000	Degreasing	VOC	Y	N	80%	60%
_____	18 005	24-20-000-000	Drycleaning	VOC	N	Y	0%	0%

FIGURE 3.5-7. EIQA AREA SOURCES SIP RULE IN PLACE CONSISTENCY CHECK

- VMT and Emissions Summary Report (assists user in performing manual examination of inventory data); and

- Emission Factors Summary Report (provides summary tables for total or time-of-day emission factors).

MOBILE model input data QA reports include:

- Geographic Consistency Exception Report (checks status of Inspection and Maintenance (I/M) programs, Anti-tampering Programs (ATP), oxygenated fuels in input files);

- I/M and ATP Control Program Consistency Exception Report (checks I/M and anti-tampering flag parameters);

- I/M and ATP Program Characteristic Range Check Exception (checks I/M, anti-tampering and fuel-related characteristics against expected values);

- Scenario Range Check Exception Report (checks model scenario inputs against expected values);

- Vehicle Speed Summary Report (provides overview of speeds used in model run; and

- Vehicle Registration Distribution Report (provides an overview of model vehicle registration distributions).

5.3.2 MOBILE INPUT DATA ANALYSIS SYSTEM (MIDAS)

MIDAS is a data processing system to facilitate the storage, retrieval, and analysis of input file variables used in mobile source modeling for SIP emissions inventories. It is designed to support evaluating the contents of MOBILE input files, which are intended to reflect all of the possible factors that could affect motor vehicle emissions within a nonattainment area.

The reports generated by MIDAS provide a convenient means of summarizing the input data and flagging potential problems. Because these data are often provided to an inventory preparer by another agency (e.g., the state's transportation department), the inventory preparer may wish to pass these reports back to the data originator for review and comment. Used in this way, MIDAS can be a useful tool to facilitate dialogue between the two agencies. Software-specific reports that MIDAS can generate are listed below:

Input File Reports

These reports provide information about the MOBILE input variables stored in the MIDAS database. Each report summarizes the information for a single database record that contains the variables for a single input file:

- Control Flag Summary (provides a synopsis of the MOBILE flag settings);

- Detailed Optional Input (provides an in-depth view of some of the optional inputs that can be modeled);

- Scenario Summary [allows user to look at contents of each individual scenario record and local area parameter (LAP) record];

- Input File Comments (provides an analysis of an input file as to its likely acceptability when used for a SIP emission inventory); and

- Input File Summary (summarizes the information contained in the previous four reports in order to provide a one-page synopsis of the input file variables and their likely acceptability for SIP modeling).

Area Reports

These reports provide information about the MOBILE input variables used to model an entire nonattainment area:

- Area Control Flag Summary (similar to Control Flag Summary);

- Area Variable Summary (presents selected parameters used to model various inventories for a nonattainment area); and

- Area Registration Summary (provides user-supplied registration distribution for each input file within the selected area).

Miscellaneous Reports

MIDAS also provides the following miscellaneous reports:

- Nonattainment Area Summary (provides a detailed description of an ozone or CO nonattainment area); and

- Database Summary (provides a listing of all the input file records that are currently in the database).

Figure 3.5-8 illustrates the use of MIDAS for a QA review of Virginia's 1990 SIP on-road mobile source inventory. The error messages summarized in the table focused the reviewer's attention on inventory data that departed from the expected (in this case, the MOBILE5a defaults). The discussion of the review provides several important pieces of information to the inventory preparer:

- The specific cause of the error flag is described;

- The relative importance of this possible error is assessed; and

- A recommended action is stated.

It should be noted that the agency did follow up on these recommendations and no errors were found.

5.3.3 VISUAL AUDITING PROGRAMS

Data visualization programs and methods can also be used as part of a QA/QC program to review data and emissions. These programs are capable of displaying the data in a more visual format (i.e., maps, timelines, scatter plots). Examples of such programs are Voyager, ARC View, and Map INFO. These software packages allow the user to browse quickly and easily through large spatial and temporal databases. Because the data are always displayed graphically, the user can see relationships that might otherwise have remained obscure or invisible. All of these packages allow the user to import data files in common formats (usually "DBF"). A linked version of Voyager, SIPView, was developed and released by the EPA specifically for use with SIP inventories.

Figure 3.5-9 shows an example from Voyager (Misenheimer, 1996). A point source emissions inventory for Georgia is plotted on a map and the relative magnitudes of the emissions are shown by the vertical bars. The circled items show sources with incorrect UTM coordinates (that is, the points are outside of state boundaries). The reviewer could check each point by displaying the data associated with each point.

If a data visualization software package is to be used as part of a QA/QC program, the following features are desirable:

- Ability to correct the data interactively will make this tool more useful for QC; that is, the user should be able to select the point, display the data, update or correct if necessary, and redisplay it.

Error Message from MIDAS Input File Comments Report	Counties/Cities Whose Input File Showed Error Message		Item Requiring Further Review	Noncritical Item
For vehicle types _____, . . . , the percentage of age 1 vehicles is high relative to the percentage of age 2 vehicles.	Charles City County Chesterfield County Chesapeake City Hampton City Hanover County Henrico County Newport City	Norfolk City Poquoson City Portsmouth City Richmond City Suffolk City Virginia Beach City York County	✓ (Norfolk City and Richmond City only)	✓ (all other cities/counties)
For vehicle types _____, . . ., the age 25 distribution is too low.	Charles City County Chesapeake City Hampton City Hanover County Henrico County Newport City Norfolk City	Poquoson City Portsmouth City Richmond City Suffolk City Virginia Beach City York County	✓	
The fraction of LDDT is too high.	Chesterfield County Colonial Heights City Hanover County	Henrico County Hopewell City Richmond City	✓	
Spikes occur in the registration distribution.	Charles City County Chesterfield County Chesapeake City Hampton City Hanover County Henrico County James City County	Newport City Norfolk City Poquoson City Portsmouth City Richmond City Suffolk City York County		✓

FIGURE 3.5-8. SUMMARY OF RESULTS FROM MIDAS REVIEW OF THE MOBILE5A INPUT FILES
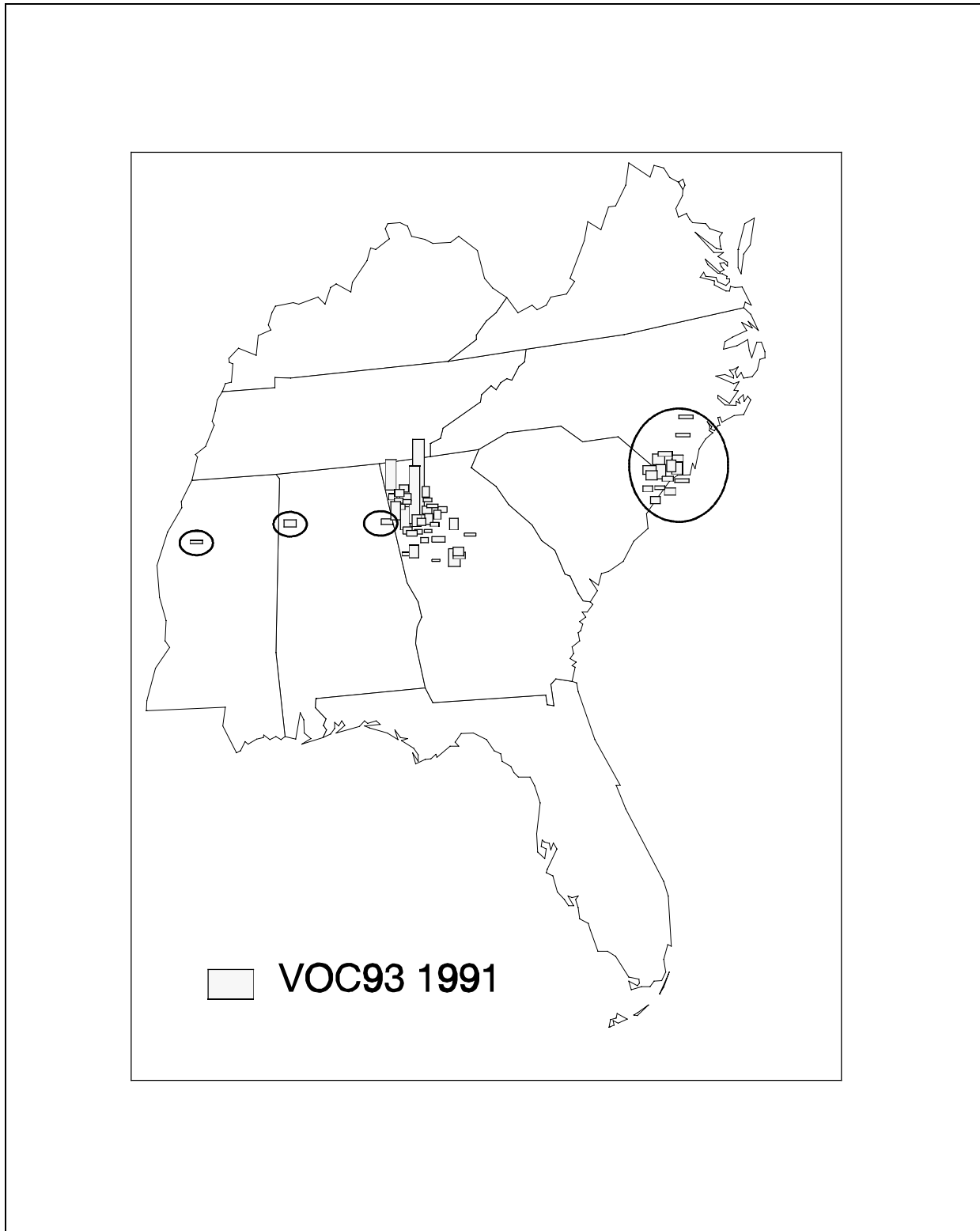
FIGURE 3.5-9. EXAMPLE OF VISUAL AUDITING TOOL

- Ability to print reports will allow easy documentation of QA/QC activities.

- Ability to print graphics will also allow documentation of QA/QC activities. Packages that only plot points are less useful than those that display values for variables associated with these points (e.g., bars representing emissions).

5.4 USER-DEFINED AUTOMATED QA CHECKS

Inventory preparers with access to computer software and the skills to fully exploit that software may wish to create their own automated QA systems. Some emissions-estimation software programs provide the user with the ability to "create" reports. This allows the user to specify what information is to be printed in a report. Alternatively, database software can be used to develop a program that will read the emissions data and generate reports. QA/QC activities can be facilitated by designing and using reports that present key variables for auditing.

A relatively sophisticated system of automated QA programs has been developed by air quality modelers in Texas (Neece and Smith, 1994). They had previously identified point source emissions as a critical component of ozone modeling and developed a series of checks, many of which are specifically designed to catch errors that will most impact modeling results (see also Section 6, "Sensitivity Analysis," of this chapter).

Two types of procedures are involved. The first is a series of database checks. One of particular interest is a ratio test. The ratio of VOC/NO_x emissions from an emissions unit is compared to the ratio of VOC/NO_x factors for that unit. Emission factors are not always used to estimate emissions, so these ratios may not always agree exactly. However, extreme disparities in the ratios are investigated (See Neece and Smith, 1994, for descriptions and examples of all tests).

The second type of procedure uses graphical analyses to plot histograms (bar charts) showing the distributions of key data. Scatter plots are also used to identify outliers (examples are shown in Figure 3.5-10). (The use of descriptive statistical methods such as these is discussed more fully in Section 7 of this chapter.) Spatial plots of the data are used to check that plant coordinates are correct.

The system of automated QA programs developed by Neece and Smith (1994) is an excellent example of an inventory QA program designed to fulfill a specific need: that of ensuring the quality of results of an air quality model that addresses issues critical to the particular modeling exercise. The developers of an inventory do not always know how their inventory will be used and, even when they know, they may not be aware of any special concerns. It is important that the *users* of an inventory identify those data quality issues and perform their own QA checks.

Figure 6. Annual Emissions vs. Stack Height

Figure 7. Log (Number of Sources) vs. Annual Emissions
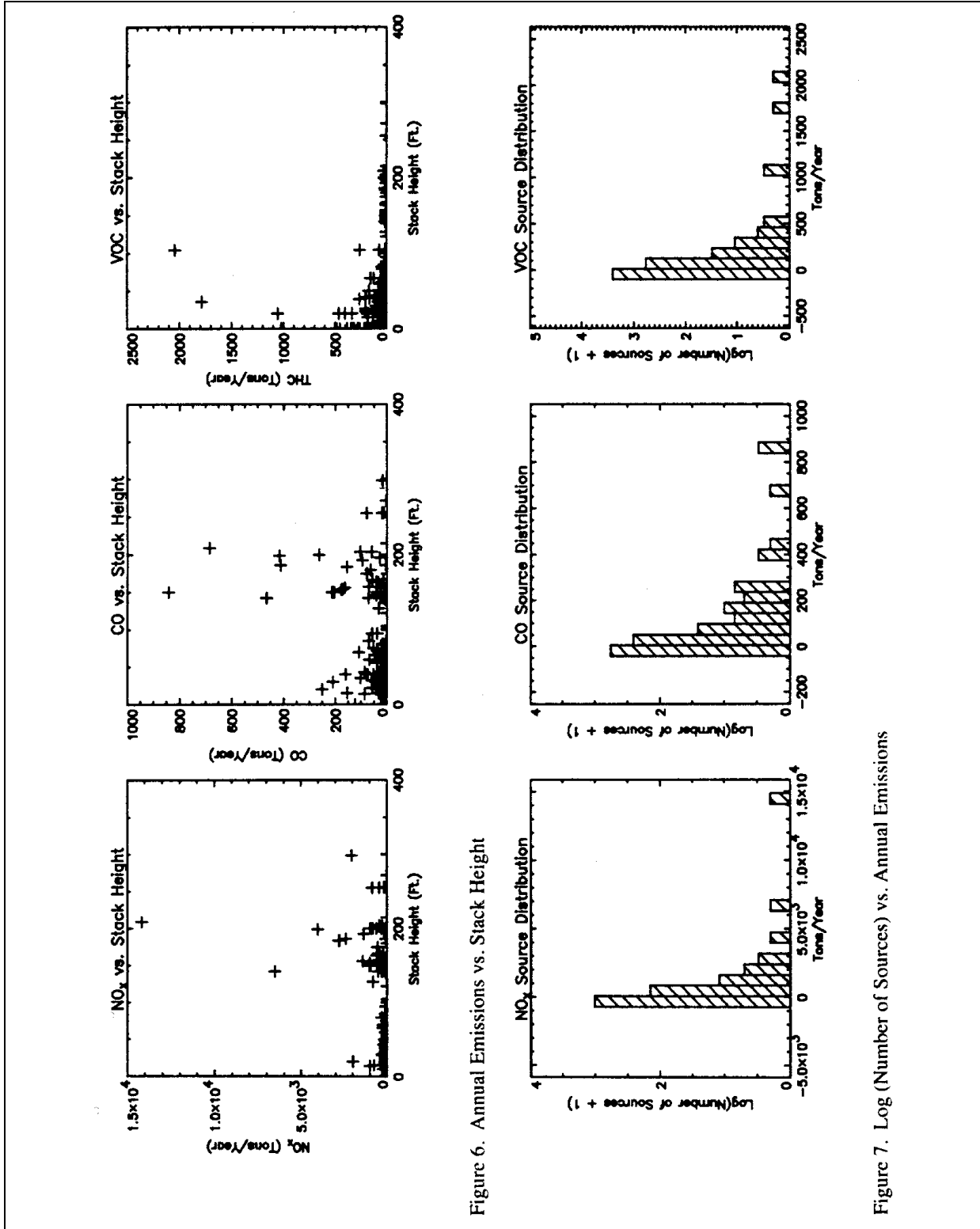
FIGURE 3.5-10. EXAMPLES OF QA SCATTER PLOTS

6

SENSITIVITY ANALYSIS

QUICK REVIEW

Definition:	A systematic study of how changes in model (or inventory) input parameters affect the output.
Objective:	To identify the parameters that have the greatest effect on the results.
Optimal usage:	When planning both the inventory and the QA program, sensitivity analysis can be used to prioritize the efforts. The user of an inventory also needs to understand the inventory sensitivities with respect to how the inventory is to be used.
Minimum expertise required:	Moderate to high, depending on model complexity and/or availability of sensitivity analysis results.
Advantages:	Allows the most efficient utilization of limited resources by focusing efforts where they will do the most good.
Limitations:	(1) Not a substitute for QA/QC procedures to verify data and calculations, and (2) can be very time-consuming if the model or inventory is very complex.

6.1 OVERVIEW OF METHOD

A sensitivity analysis is a process for identifying the magnitude, direction, and form (e.g., linear or nonlinear) of the effect of an individual parameter on the model's result. It is usually done by repeatedly running the model and changing the value of one variable while holding the others constant. If a model has a large number of variables, conducting a thorough sensitivity analysis can require a great deal of effort.

With respect to emissions inventories, sensitivity analyses may be used to: (1) evaluate the overall inventory, (2) identify sensitivities of specific emissions models, or (3) identify key inventory data that, when used as input to air quality models, have the potential to significantly affect the results. These types of analyses should be used when planning an inventory in order to focus both development resources and QA/QC efforts on the critical elements of the database. Sensitivity analyses will also be important to the user of the final inventory.

Sensitivity analyses of inventories can be accomplished through several steps, and even the simplest approach can yield useful results. For example, individual source categories can be ranked in order of their contribution to total emissions for a given pollutant. A variation is to rank the categories and then calculate the cumulative percent of emissions. These ranks can then be used to prioritize categories and target the QA efforts.

Somewhat more complicated, but also more useful, is identifying the impacts of underlying variables on emissions. For example, population is a commonly used surrogate for calculating area source emissions of VOCs. If area sources are a large component of a VOC inventory, small errors in the population value can have a significant impact on the emissions estimate. Knowledge of this fact might prompt an agency to conduct a survey or to use methods other than per capita factors.

Models are often used to estimate emissions for specific source categories. Table 3.6-1 lists many of these models and provides references for some publicly-available sensitivity analyses. Unfortunately, complete sensitivity analyses have not been published for many of these models.

It is ultimately up to the inventory developers to determine the significance of each source category in their inventories and direct QA efforts accordingly. If a source category contributes a relatively small proportion of the emissions, conducting a sensitivity analysis may not be worthwhile.

TABLE 3.6-1

KEY VARIABLES FOR SOME EMISSIONS ESTIMATION MODELS

Model	Description	Key Variables
MOBILE5b[a]	Mobile source emission factors	I/M, VMT mix, speed, mileage accumulation, temperature
BEIS, BEIS-2.2[b]	Biogenic emissions	Canopy effects, temperature, sunlight, biomass/land-use
Landfill Air Emissions Estimation Model[c,d]	Landfill VOC and methane emissions	Decay rate (k), methane potential of waste (L_0), nonmethane organic compound (NMOC) concentration, length of time refuse has been in place
SIMS[d]	VOC emissions from wastewater treatment	Aeration, biodegradation, surface area and wind speed, retention time
TANKS[d]	Emissions of organic liquids from fixed-roof or floating-roof tanks	Location, tank type, tank contents

[a] From data supplied by Office of Mobile Sources; for more discussion, see the example in this section.
[b] Pierce et al., 1990; Birth, 1995; see also Lamb et al., 1993; Gaudioso et al., 1994.
[c] Peer et al., 1992.
[d] From Session 10 of "Emissions Inventory Satellite Workshop Training Manual/Presentation Material."

Finally, if the inventory is being prepared as input for a model, a sensitivity analysis of that model can be very useful for inventory preparation and QA. Table 3.6-2 lists several air quality models that require emissions inventories as input. Although ensuring the accuracy of emissions is obviously important for all these models, the importance of other inventory parameters varies from model to model. The relevant temporal scale, for example, may be annual, daily, or hourly, and the maximum or the average emissions may be required. Spatially allocating emissions presents an additional complication. Some models for some pollutants may be very sensitive to spatial scales; for example, models of tropospheric ozone formation may be very sensitive to the spatial distribution of short-lived pollutants, but relatively insensitive to those with longer half-lives. Table 3.6-3 summarizes the preferred and alternative methods for using sensitivity analyses in the development of emissions inventories.

TABLE 3.6-2

KEY INVENTORY VARIABLES FOR SOME AIR QUALITY MODELS

Model	Scale[a]	Key Inventory Variables
Industrial Source Complex Long Term (ISCLT)	Local (up to 20 km), annual concentrations	• Emission rates • Point source plume rise[b] • Location of source(s) • Dimensions of buildings adjacent to sources
Industrial Source Complex Short Term (ISCST)	Local (up to 20 km), hourly, 8-hour, 24-hour	
Urban Airshed Model (UAM)	Urban (20 to 200 km), hourly	• Location of point sources • Spatial/temporal allocation of area and mobile source emissions • Emission totals per grid cell • Point source plume rise[b] • Speciation of VOC compounds • Temperatures (used to estimate biogenic emissions)
Regional Acid Deposition Model (RADM) and Regional Oxidant Model (ROM)	Regional (200 to 2000 km), hourly	• Location of point sources • Point source plume rise[b] • Speciation of VOC compounds

[a] Spatial scale conventions from NAPAP (1991) are used here.

[b] Inventory variables used to calculate plume rise are exit velocity, exit temperature, and stack diameter.

<div align="center">

TABLE 3.6-3

SENSITIVITY ANALYSES: PREFERRED AND ALTERNATIVE METHODS

</div>

Method	Procedure
Preferred	When preparing the Inventory Preparation Plan (IPP/QAP) for an emissions inventory, prioritize data gathering and QA/QC efforts by conducting sensitivity analyses to focus on key variables. The analyses should include: (1) previous inventories, (2) emissions models to be used in preparing the inventory, and (3) models for which the inventory will be used as input data.
Alternative 1	Use existing sensitivity analyses of emissions models and of previous inventories to identify key variables and potential trouble spots.

6.2 SENSITIVITY ANALYSIS FOR AN AREA SOURCE INVENTORY

Area source emissions are often estimated using an emission factor and a surrogate for the emissions activity. Population and employment by SIC code category are commonly used in this approach. As discussed in Chapter 1 of Volume III (Preferred and Alternative Methods for Area Sources), the use of these surrogates is a significant source of uncertainty of the emissions.

Table 3.6-4 shows the percent of VOC emissions attributable to specific area sources for a state and the methods used to estimate the emissions. A large percentage of the emissions were estimated using per capita or per employee factors. To determine just how important population and other surrogates are to the overall estimate, a simple sensitivity analysis was conducted.

The sources were assigned to six general methods groups: (1) per capita, (2) per employee, (3) throughput (this includes any category for which emissions are based on fuel use, production, or consumption of a material), (4) statistical models, (5) surveys, and (6) engineering judgment. Based on expert judgment, the ranking of the estimates from highest to poorest quality was:

1.   Survey

2.   Throughput

3.   Statistical models

TABLE 3.6-4
DAILY VOC INVENTORY FOR A STATE

Area Source Category	VOCs, lb/day	% Total	Estimation Procedure
Commercial/Consumer Solvent Use	302,854	18	per capita
Architectural Surface Coating	295,558	17	per capita
Gasoline Distribution	246,175	14	gasoline consumption
Industrial Surface Coating	240,237	14	per employee, per capita
Surface Cleaning Operations	172,429	10	per employee
Dry Cleaning Operations	73,904	4	per employee
Petro. Vessel Loading/Unloading	66,673	4	petro products loaded/unloaded
Automobile Refinishing	51,931	3	per capita
Graphic Arts Facilities	48,037	2	per capita
Asphalt Paving	32,450	1	consumption
Traffic Paints	28,976	1	per capita
Agricultural Pesticides Application	22,421	1	application rate, acres crops
Commercial Bakeries	20,654	1	per capita
Structure Fires	18,728	1	per fire
Municipal Landfills	13,496	0	statistical models
Residential Fuel Combustion	4,571	0	fuel use
Industrial Fuel Combustion	3,775	0	fuel use
Aircraft Refueling	2,111	0	aviation fuel consumption
Apartment Incinerators	563	0	engineering judgment
Wastewater Treatment	462	0	survey
Hospital Sterilizers	299	0	per hospital bed
Forest Fires	292	0	acres burned
Commercial/Institutional Fuel Combustion	266	0	fuel use
Breweries	192	0	state beer production
Barge, Tank Car, Rail Car, Drum Cleaning	119	0	survey, engineering judgment
Medical Waste Incinerators	11	0	engineering judgment
Asphalt Roofing Kettles	1.5	0	per square paper
Orchard Heaters	0	0	survey
Distilleries	0	0	survey
Agricultural/Slash Burning	0	0	survey
Wineries	0	0	state wine production
Open Burning	0	0	survey

4.   Per employee

5.   Per capita

6.   Engineering judgment

(For more discussion on emissions quality ranking and/or uncertainty, see Chapter 4 of this volume.)

Figure 3.6-1 is a histogram of percent VOC (from Table 3.6-4) estimated by each of the above methods. An important finding of this simple analysis is that over 70 percent of the area source VOC emissions were estimated using two mid- to low-quality methods. The state air pollution control agency is seeking ways to reduce emissions, and viable control methods have been identified for some coatings. The Agency now is concerned that more accurate methods may be needed to evaluate the effects of controls for these population-based estimates.

Because emissions were estimated using mostly linear models (e.g., emission factor times activity), the relationship between the emissions estimate and population and/or employment is easy to understand. Figure 3.6-2 demonstrates how percentage changes in population or employment affect VOC emissions. The graph shows that a 25 percent change in population will result in a 10 percent change in *total* area source VOCs (that is, VOCs from all sources). This suggests that small errors in the population variable do not have a very large impact overall. If the inventory preparer has alternative estimates of population (or other variable used as activity data), an analysis such as this can help determine whether the choice of alternative values is a significant one.

This type of analysis can be used to target area source categories for improvement. In this example, the state agency's plans for the next inventory might include:

•   Dropping the "Open Burning" and "Barge Cleaning" categories because surveys showed these were not important sources of emissions;

•   Conducting a survey of paint distributors to develop more reliable estimates for "Architectural Surface Coating;" and

•   Intensifying point source surveys to cover more of the industrial surface coating emissions in the point source inventory and using data from smaller sources to develop local per employee factors.
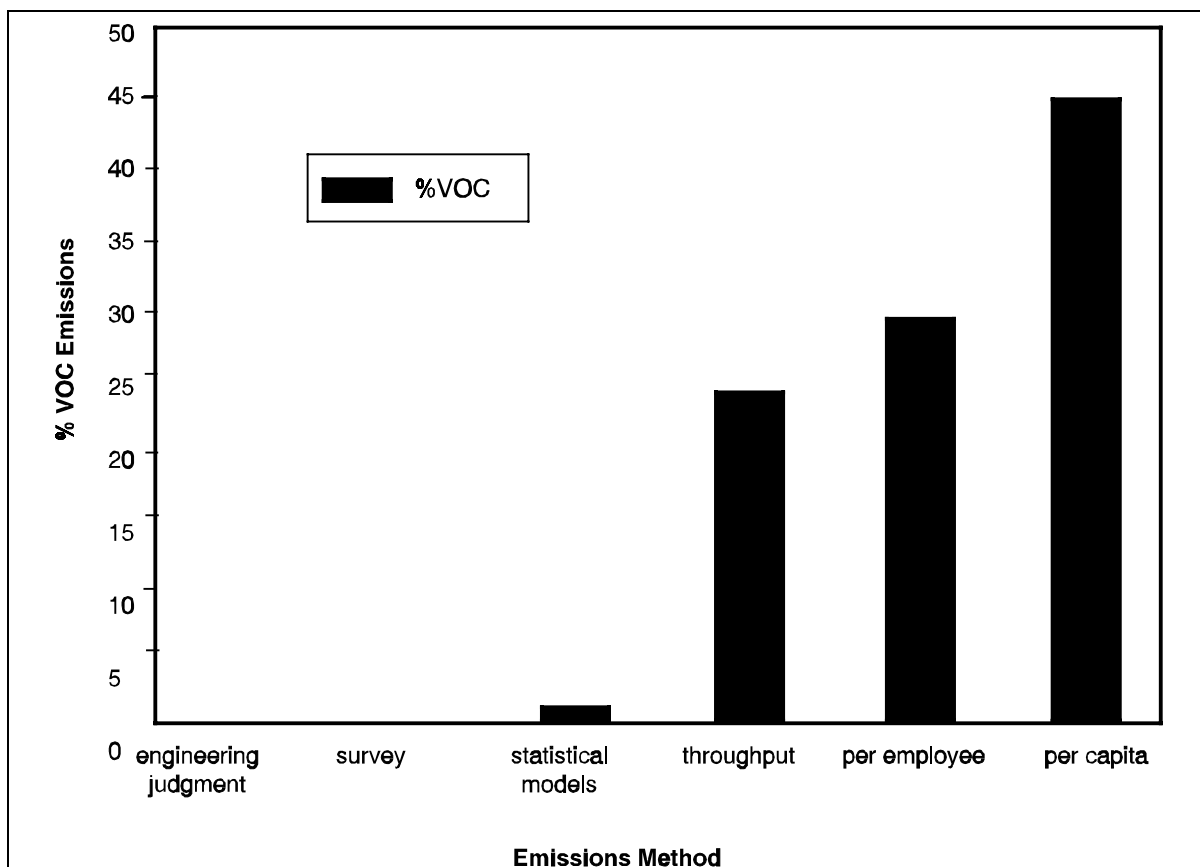
FIGURE 3.6-1. PERCENT VOC BY ESTIMATION METHODOLOGY

This is a very simple example of a sensitivity analysis. Its simplicity is a result of the methods used to estimate emissions. As more complicated methods are used, the complexity of the analysis increases. Also, specific results from this analysis cannot necessarily be extrapolated to other inventories. Each inventory has unique features and sensitivity analyses need to be conducted to meet specific objectives.

6.3 SENSITIVITY ANALYSIS OF EPA'S MOTOR VEHICLE EMISSION FACTOR MODEL

The EPA's MOBILE model is the most commonly used method for estimating onroad mobile source emission factors. At the time this volume was written (1997), version 5b of the model was in use. A fairly detailed sensitivity analysis of version 4.1 was conducted in 1992 and the results distributed by the EPA's Office of Mobile Sources (OMS). One example from that analysis is presented here.
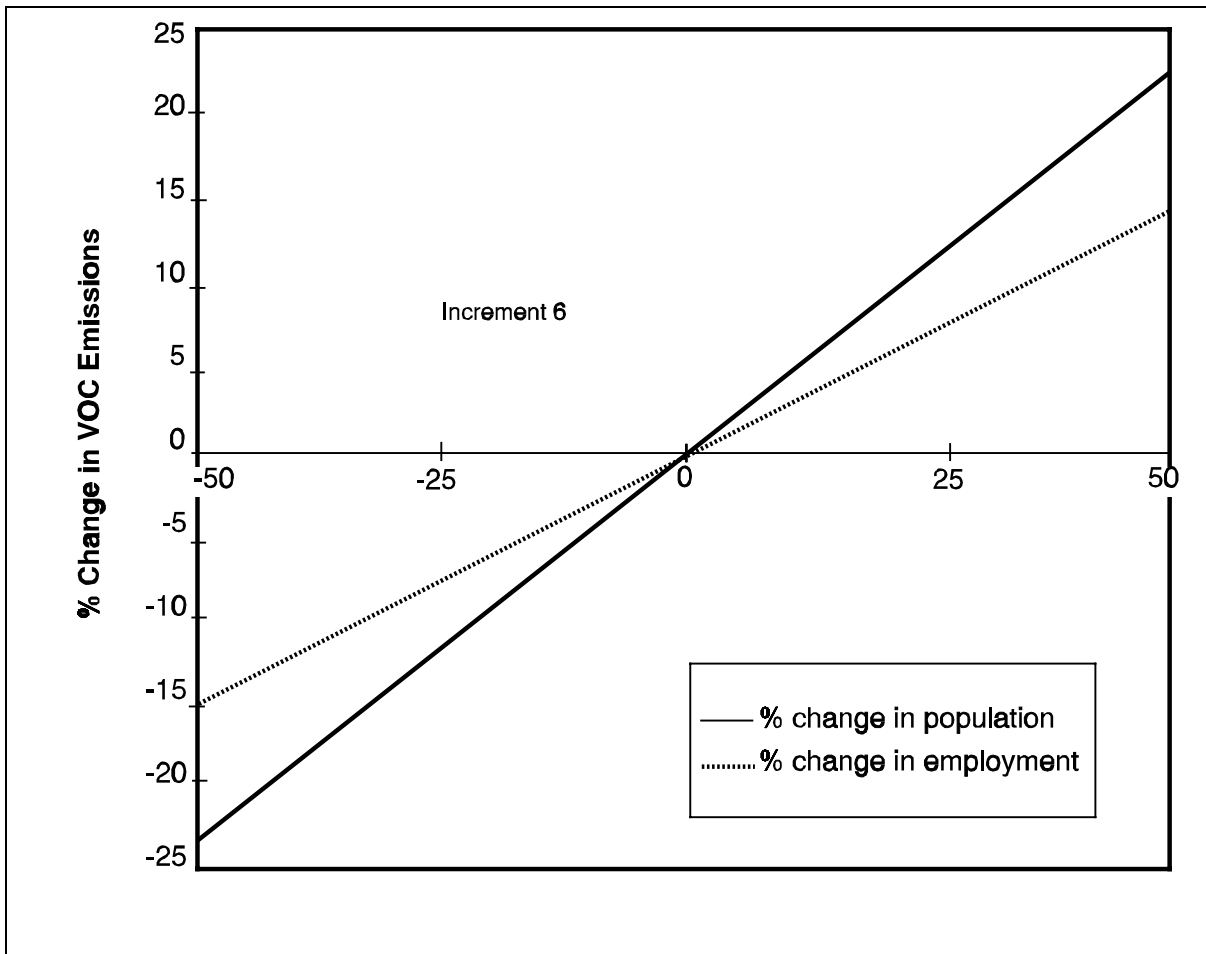
FIGURE 3.6-2. EFFECT OF POPULATION, EMPLOYMENT ON AREA SOURCE VOCS

The MOBILE model is one of the most complex models commonly used for emissions estimation. Default data are provided for many of the input variables, but the user is encouraged to develop region-specific input data.

This sensitivity analysis compared three test cases. The conditions used for each case are summarized in Table 3.6-5. The results of the analysis for nonmethane hydrocarbon (NMHC) emissions are summarized in Figure 3.6-3a. Not surprisingly, VMT has a significant linear effect on emissions. Just as in the area source example described previously, emissions are estimated by multiplying a factor by an activity value (i.e., VMT). The other variables, however, directly affect the emission factors produced by the MOBILE model. The model was relatively insensitive to changes in Vehicle Age Distribution and VMT mix (less than 5 percent difference in emissions). Other variables had a more profound effect; for example, underestimating the average speed by as little as 5 miles per hour (mph) resulted in greater than a 20 percent increase in emissions.

TABLE 3.6-5

MODEL INPUT VALUES USED FOR MOBILE4.1 SENSITIVITY ANALYSIS

Variables	Range of Conditions			Notes
	Low	Base	High	
Inspection/ Maintenance (I/M)	Basic	None	High option enhanced	Indicates the effects of I/M options.
Travel (VMT)	75,000	100,000	125,000	A percent change in VMT causes the same percent change in emissions.
Speed (mph)	14.7	19.6 FTP speed	24.5	Indicates the effect of inputting an incorrect speed.
Temperature (°F)	65-90	70-95	75-100	Indicates the effect of a 5°F error in temperature.
Hot/Cold Distribution PCCN/PCHC/PCCC	5.0/5.0/5.0	20.6/27.3/20.6 FTP cycle	5.0/55.0/5.0	The low condition represents fewer hot or cold starts than the FTP cycle. The high condition represents an increase in hot starts, but few cold starts.
VMT Mix	Fairbanks	MOBILE4.1 default	California	In Fairbanks more VMT is distributed to heavy duty gasoline and diesel trucks than in the MOBILE4.1 default. California has more VMT distributed to cars and heavy duty gasoline trucks.
Mileage Accumulation	Fairbanks	MOBILE4.1 default	California	The low mileage accumulation in Fairbanks on light duty autos was substituted for the MOBILE4.1 default for the low condition. California mileage accumulation is greater than the MOBILE4.1 default.
Vehicle Age Distribution	Fairbanks	MOBILE4.1 default	Phoenix	The Fairbanks vehicle fleet has a smaller percentage of older cars while Phoenix has a larger percentage than the MOBILE4.1 default.

FTP = Federal test procedure
PCCN = % of VMT accumulated by non-catalyst-equipped vehicles in cold-start mode.
PCHC = % of VMT accumulated by catalyst-equipped vehicles in hot-start mode.
PCCC = % of VMT accumulated by catalyst-equipped vehicles in cold-start mode.
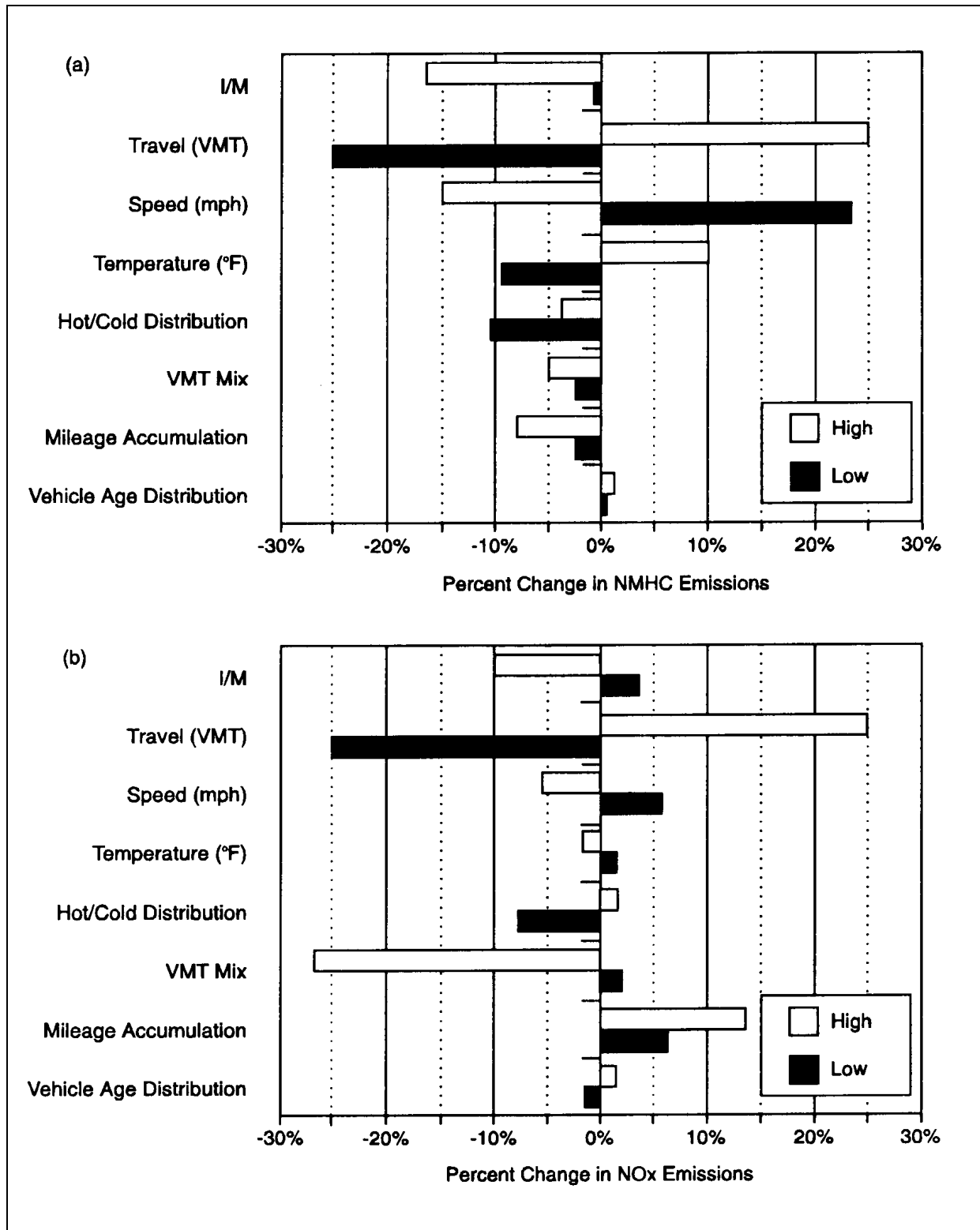
FIGURE 3.6-3(A AND B). SENSITIVITY OF NMHC, NO$_X$ EMISSIONS

However, as Figure 3.6-3b shows, model sensitivities are different for other pollutants. VMT mix is very important for summertime NO_x emissions, but temperature is not (These results are based on the same set of conditions as those in Figure 3.6-3a).

These sensitivity studies of the MOBILE model illustrate the importance of analyzing the model for all potential scenarios of interest. Pollutants may be affected differently by changes in variables; also, the time of the year may be an important factor.

6.4 SENSITIVITY OF AIR QUALITY MODELS TO INVENTORY INPUT DATA

The users of inventories often have little or no involvement in developing the inventory. Therefore, they may subject the inventory to intensive review and specific QA procedures designed to identify problems that could impact the outcome of their particular use of the inventory. One such group is composed of air quality modelers.

Air quality modelers typically conduct sensitivity studies of the air quality model response to changes in emissions data input to the model. These sensitivity studies many times are simple and involve across the board increases or decreases in total emissions. For example, a common sensitivity simulation usually performed for most photochemical modeling studies is the removal of all emissions from the simulation. These bounding simulations, while not realistic, provide the modeler with information as to the overall response of the photochemical model to changes in emissions.

While very useful for interpreting modeling results for a given modeling domain, emission sensitivity simulations *cannot* be generalized to all photochemical modeling studies. Every modeling study will have its own peculiarities and results of sensitivity simulations for the region cannot be extrapolated to other areas. The meteorology for a region, the magnitude and relative mix of biogenic, area, and point source emissions, the reactivity of the emissions, the initial and boundary conditions in the region, and the occurrence or non-occurrence of transport of precursor pollutants from outside the domain all combine to create a set of unique responses to changes in emissions in a given modeling domain.

With the above caveat in mind, it is still useful to examine the type of information that can be obtained from a properly formulated sensitivity study. Below are three examples of the type of information feedback to the inventory specialist that can result from sensitivity studies.

SOUTHERN CALIFORNIA

Numerous investigators have examined the sensitivity of ozone formation to emissions in the South Coast Air Basin (Los Angeles metropolitan area) in Southern California. A key driver for these emission sensitivity studies was the results of the tunnel study of motor vehicle emissions conducted during the Southern California Air Quality Study (SQAS) (Pierson et al., 1990). The results of this study indicated that onroad motor vehicle hydrocarbon emissions were significantly underestimated in the South Coast Air Quality Management District (SCAQMD) inventory. The SCAQMD addressed this issue in its 1994 Air Quality Management Plan (AQMP) by conducting photochemical model sensitivity studies in which hydrocarbon emissions from all onroad vehicles were doubled (SCAQMD, 1994). The SCAQMD modeling was performed using the Urban Airshed Model (UAM). For all episodes modeled, model performance for the doubled vehicle hydrocarbon emissions scenario was significantly improved above the base case.

Harley et al. (1993), using the California Institute of Technology (CIT) photochemical model for the same Los Angeles episodes, also adjusted upward motor vehicle emissions as indicated from the SCAQS tunnel study results. Again, there was a significant improvement in model performance using the upward adjusted motor vehicle emissions inventory. Results from these two modeling studies using different models and methodology provide significant insight into potential biases in the 1994 AQMP motor vehicle emission inventory and demonstrate the value of emission sensitivity studies.

TEXAS GULF COAST

A different type of emissions sensitivity analysis was performed by Neece and Smith (1994) using UAM simulations for the Texas Gulf Coast. The automated QA program developed by Neece and Smith has been previously discussed in Section 5 of this chapter. In their sensitivity analyses, they examined the sensitivity of peak ozone concentrations to individual components of the emission inventory. Based upon these analyses, they concluded:

- Peak predicted ozone concentration is more sensitive to point source emissions than to area, mobile, or biogenic source emissions.

- "Hot spots" in the grid occur where NO_x and VOC emissions are mixed; these grid cells need to be checked carefully to ensure that point source locations are correct.

- The emissions from large sources outside the boundary of the modeling domain are not detected by UAM; therefore, a test was designed to identify large sources just outside the upwind boundary.

As a consequence of their concern over these model sensitivities, Neece and Smith developed their own automated QA procedures to review point source inventories.

ATLANTA

Biogenic emissions are a very significant source of hydrocarbon emissions in the Atlanta, as first reported by Chameides et al. (1988). In a subsequent analysis of biogenic emissions in the Atlanta area, Cardelino (1995) analyzed the impact on ozone precursor emissions and ozone concentrations of changes in land use patterns, alternative estimates of isoprene emissions from biogenic sources, and variation in temperature reflecting different land use patterns. Based on this analysis, Cardelino concluded:

- There remains uncertainty in the most appropriate algorithm for estimating biogenic emissions of isoprene, a highly reactive component of biogenic emissions.

- Satellite imagery can potentially provide improved representation of temperature fields, leading to improvements in the temporal distribution of emission inventories and to potential improvements in modeled ozone concentrations.

- Future population changes and urbanization can significantly change land use with resulting changes in ambient surface temperatures. These changes should be taken into account when developing future year emissions estimated and when performing photochemical modeling simulations.

The above studies reflect a sample of the information feedback available to the inventory specialist from the performance of photochemical modeling emission sensitivity studies. Again, each sensitivity result cannot be reliably extrapolated outside the specific modeling domain for which the results were obtained. However, the inventory specialist is encouraged to work with the end-users of inventories to design the appropriate sensitivity studies for a given area and inventory. By gaining an appreciation of the ultimate uses to which an inventory is subjected, end-use concerns can be addressed when planning the inventory, preparing the QAP, and in subsequent inventory development and QA/QC activities. The active involvement of the inventory specialist with the end-use of the inventory will tend to minimize additional analyses and QA that modelers and other end-users perform to better understand the inventory.

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7

STATISTICAL CHECKS

QUICK REVIEW

Definition:	The use of descriptive statistics, or statistical tests or procedures to evaluate or control data quality.
Objective:	Descriptive statistics are most commonly used to compare results, and to flag unusual or unlikely values. More formal statistical procedures may use specified sampling methods and performance specifications as a quality control procedure.
Optimal usage:	Descriptive statistics are useful for QA as part of a Peer Review or Independent Audit of a completed or partially completed inventory; particularly useful for comparing different inventories. Statistical QC is potentially a very useful method for inventory QC.
Minimum expertise required:	Moderate to high, depending on how much the system is automated, and the complexity of the analysis.
Advantages:	(1) Can process large amounts of data, (2) can reduce subjectivity of informal reality checks, and (3) contributes to the continuous improvement of inventories.
Limitations:	(1) More sophisticated methods require some understanding of statistical theory, (2) common statistical methods are based on assumptions of normality (which is often not the case for emissions data), and (3) not a replacement for human evaluation and judgment.

7.1 OVERVIEW OF METHODS

Statistical procedures offer a wide array of tools that perform many of the same QA/QC functions described in previous sections. As with the automated checks discussed in Section 5, statistical checks are generally used as a tool to facilitate reality checks (Section 2), peer reviews (Section 3), or independent audits (Section 8). They are also used in some emissions validation procedures (Section 9). Many of the statistical methods described in this system can be automated, and probably should be if the data sets are very large or if the procedure is to be repeated many times.

There are two basic methods used to draw conclusions about data quality; the most commonly used does not require statistical analyses. For example, the usefulness of reality checks stems from the reviewer's ability to examine or compare some values, and to draw a conclusion from them. The reviewer is using *logical inference* to draw that conclusion; that is, the facts are weighed against that reviewer's knowledge of the subject and a conclusion about the validity (this process may also be called engineering judgment or expert judgment). *Statistical inference* is an alternative method for drawing conclusions about data sets. For some types of decisions, statistical inference is more trusted and more reliable than logical inference. However, this is not necessarily true in all situations. Sometimes the answer is so obvious that statistics are not needed. Also, often too little is known about the data distribution to use statistical procedures reliably.

If statistical checks are only alternative ways of performing the other procedures described in this document, it is reasonable to ask why statistics should be used at all. The non-statistical approach to QA/QC requires the reviewers to base their decisions on their experiences with inventory preparation (which includes knowledge of past quality history) and on their understanding of the weaknesses in the data, methods, and process. This approach is sound in principle, but is also subject to several potential problems. The experts' memories may be inaccurate or short; furthermore, key experts may leave the agency, taking this "institutional knowledge" with them. Reliance on historical problems may lead to a failure to identify new problems in unexpected areas. Finally, experts are sometimes wrong; the uncritical acceptance of an expert's value can lead to persistent errors. While it is impossible to fully automate a QA/QC program and not advisable to rely entirely on statistical methods, the use of statistical descriptors, analytical procedures, and random sampling should be used to decrease reliance on key experts. Also, some institutional knowledge can be built into the statistical procedures.

The term *statistical checks* as used in this section describes a miscellaneous set of tools/procedures that are mostly useful for QA but can sometimes be applied to QC as well. However, many of these procedures fit the concept of "statistical quality control." This is the label attached to a formal system of process QC founded by W.A. Shewhart in the 1930s and popularized by W.E. Deming in the second half of the 20th century. Although originally

applied to manufacturing processes, the concept has been expanded to cover services as well. While formal statistical QC procedures have not been widely applied to emissions inventories, QA/QC procedures such as the range checks described under "Computerized Checks" (Section 5) are very similar to the acceptance sampling procedures used in statistical QC. The procedure could be extended to emissions inventories in the future, and some useful concepts from statistical quality control are included in this section.

Commonly used statistical methods for inventory QA/QC are:

1. Descriptive statistics (mean, standard deviation, frequency distributions, etc.) are often used for data presentation and to facilitate peer review (see Section 7.2).

2. Statistical procedures to detect outliers can be used for range check procedures (see Section 7.3).

3. Statistical tests (such as t-tests or similar analyses) can be used for comparability checks (to compare two or more inventories) and for data validation, such as comparing inventory data to ambient data, or evaluating the relationships between parameters used in an inventory (see Section 7.4). The latter is discussed in more detail in Section 9.

The first two types of methods are used fairly commonly; the third method has not been used very much but probably should be.

Because statistical analysis requires specialized expertise and also because essential QA/QC functions can be met using non-statistical methods, the EIIP has not designated any preferred or alternative statistical methods. The information in this section is provided to assist those who wish to incorporate statistical methods in their inventory QA/QC program. Also, if surveys and/or statistical methods are used to develop emission inventories, this section will be useful to peer reviewers or QA personnel who need to assess the validity of the statistical methods used. However, only an overview of important statistical terms and concepts is provided; for more detailed information, the reader should consult the references cited in this volume.

7.2 DESCRIPTIVE STATISTICS

The most common use of statistics in emission inventories is to summarize and report both emissions and the data used in calculations. However, statistics are useful at several stages in the inventory process. They can be used to make informed decisions about the appropriate data or model to use, and to document the reasons for that choice. They are used to screen large datasets or emissions calculations to identify potential errors. Statistical

descriptors are also useful for assuring consistency within an inventory. For example, when comparing emissions from different counties, a greater than expected range of emissions for one county may be shown. These would be flagged for further checking of the data and methods.

Table 3.7-1 summarizes descriptive statistics that are useful for these purposes. QA reports (such as some of those shown in Section 5) can and do make use of summary statistics to facilitate peer review of the database. Statistics used in this way are primarily useful as a screening method much like a reality check. They should also be used to report and document the data (as discussed in Chapter 2, reporting and documentation play an important role in QA). While it may be difficult to spot an unusually large value in a vast data array, that number should stand out if the proper summary statistics are displayed.

One major limitation in advancing the use of statistical methods for QA/QC of inventories is that there has been little published analysis of the statistical characteristics of emission inventories. There is a general recognition that the frequency distributions of emissions are often not normal (or Gaussian). The lognormal distribution is held to be more representative of emissions data. However, the emission source, the type of pollutant, and the basis on which emissions are being presented (e.g., per Btu, per unit fuel, per capita, etc.) will determine the resulting distribution. If statistical methods (even the simple methods are described here) are to be used effectively, the expected distribution (i.e., the one that should occur if everything is correct) needs to be known. This will become the reference distribution that can be used as the basis for comparison.

TABLE 3.7-1

COMMONLY USED STATISTICAL DESCRIPTORS

Term	Formula	Explanation
Observation	x_i	The variable or attribute being measured.
Sample size	n	The number of values (or x_i's) in a set.
Arithmetic mean	$\overline{x} = \dfrac{1}{n} \sum\limits_{i=1}^{n} x_i$	The mean, or average, is the most commonly used estimate of central tendency. However, it is very sensitive to extreme values and is not a good measure if there is a very skewed distribution or very large outliers.
Range	$R = x_{max} - x_{min}$	The span of a set of numbers where x_{max} is largest number and x_{min} is smallest number in set. The range is most useful when emissions data are highly uncertain and an expert is using judgment to place "bounds" on the expected values (e.g., "fugitive dust emissions from unpaved roads are between a range of 0.25 and 3.0 times the value estimated using method x").
Variance of a sample	$s^2 = V = \dfrac{\Sigma(x_i - \overline{x})^2}{n - 1}$	A measure of the variability in a sample.

TABLE 3.7-1

CONTINUED

Term	Formula	Explanation
Standard deviation of a sample	$s = \sqrt{V}$	A measure of dispersion in the original units (e.g., tons per year), The standard deviation, along with the mean, are the principal measures used to define a value such as an emission rate and the associated uncertainty in the value. For normally distributed data, approximately 95 percent of values lie within ±2 standard deviations of the mean.
Estimated sum of population	$N\bar{x}$	The estimated sum of x_i's in the population of size N; this formula should be used to estimate area source emissions from a survey of a representative sample of sources.
Standard error of the estimated sum	$s_{N\bar{x}} = \frac{Ns}{\sqrt{n}} \left(\sqrt{1 - \frac{n}{N}} \right)$	The estimated error associated with the sample used to estimate the population sum. The value of s is the sample standard deviation as defined above. Note that as n approaches N, the error of the estimated sum approaches zero.
Median	The value x_i such that there is an equal number of values larger and smaller.	The median is the value from a sample with a cumulative frequency of 50 percent. It is relatively insensitive to extreme values so is a good measure of central tendency when there are extreme values such as is the case for most ambient monitoring data.

TABLE 3.7-1

CONTINUED

Term	Formula	Explanation
Percentile	---	The value on a scale of 100 that indicates the percent of a distribution that is equal to or below it.
Geometric mean	$$\overline{y} = \exp\left(\frac{1}{n} \sum_{i=1}^{n} y_i\right)$$ where $y_i = \ln x_i$	Many environmental parameters such as air quality monitoring data tend to obey a lognormal distribution rather than a normal distribution. Consequently, the logarithmic transformation of $y_i = \ln x_i$ allows the data to be treated as if coming from a normal distribution.
Confidence interval of sample mean of sample proportion (p)	$$\overline{x} - t_{\alpha/2,\, n-1}\ s/\sqrt{n}$$ $$\overline{x} + t_{\alpha/2,\, n-1}\ s/\sqrt{n}$$ $$p - t_{\alpha/2,\, n-1} \sqrt{\frac{p\,(1-p)}{n}}$$ $$p + t_{\alpha/2,\, n-1} \sqrt{\frac{p\,(1-p)}{n}}$$	Values used to estimate a statistical parameter and that tend to include the true value of the parameter a predetermined proportion of the time if the process of finding the group of values is repeated a number of times. A confidence interval provides an estimate of the upper and lower bounds of a value at a given level of confidence (e.g., there is a 95 percent certainty that another sample would produce an estimate between the upper and lower bounds).

TABLE 3.7-1

CONTINUED

Term	Formula	Explanation
Absolute bias	$B_{abs} = \bar{x} - Obs$	The bias in an emissions estimate or parameter is the difference between the estimated value and the "true" value that is "known" through measurement or observation. The absolute bias is appropriate when the bias is relatively constant across all estimates of the true value (e.g., an incorrect offset voltage in a data logger produces a constant offset in the measured temperature).
Relative bias	$B_{rel} = \dfrac{\bar{x} - Obs}{\bar{x}} \times 100$ $B_{rel} = \dfrac{\bar{x} - Obs}{Obs} \times 100$	The relative bias is the absolute bias expressed as a percentage of either the "true" value or the estimate. It is more appropriate than the absolute bias when the magnitude of the bias is a function of the value itself (e.g., the bias in estimates of VOC emissions from motor vehicles is a function of estimated vehicle miles travelled).
Coefficient of variation	$CV = \dfrac{s}{\bar{x}} \times 100$	The coefficient of variation expresses the standard deviation as a percentage of the mean value. For lognormally distributed data such as most ambient monitoring data, the coefficient of variation is used analogously to the standard deviation.

TABLE 3.7-1

CONTINUED

Term	Formula	Explanation
Root of the mean squared error	$$RMSE = \sqrt{\sum_{i=1}^{n} \frac{\left(x_i - Obs\right)^2}{n}}$$	The root mean squared error expresses the variability in the bias in a form analogously to the sample standard deviation. The RMSE can be used analogously (but not equivalently) to the standard deviation or coefficient of variation to express uncertainty.

where:

    t   =   Student's t distribution;

    α =   significance level; and

    Obs =   observed emission value of the "true" value of the parameter.

Most of the statistical measures shown in Table 3.7-1 apply to data that obey a normal distribution. However, emissions data tend to not be normally distributed for a number of reasons including:

- Emission inventories can be dominated by a few very large sources (i.e., utility NO_x and sulfur oxides (SO_2) emissions);

- The underlying activity data used to estimate emissions are not typically normally distributed (e.g., vehicle mile traveled data, population density in an urban area); and

- The processes that lead to elevated emissions tend to be driven by extreme events that are not normally distributed (e.g., high load and acceleration events for motor vehicle, out of specification sulfur content for fuel oil, high wind speeds for wind blown dust).

Consequently, an inventory specialist should evaluate the emissions data for normality prior to any detailed statistical analysis of the emissions data or its uncertainty. The objective of this section is to discuss methodology available for assessing the distributional nature of emissions data.

Emissions from point sources are also often lognormal when expressed on a per facility basis. The distribution of businesses based on size (where size is measured by number of employees) is a well-documented example of a lognormally distributed variable (Lawrence, 1988). For those industries where emissions are correlated with number of employees, the distribution of emissions is at least partly explained by this fact.
Furthermore, for area sources whose emissions are estimated using per employee factors, a lognormal (or other non-symmetrical) distribution of emissions is to be expected.

Some data distributions relevant to emissions inventories are shown in Table 3.7-2. While it is not necessary to understand the underlying mathematics, it is important to recognize that many common statistical procedures are based on the assumption of normality. However, real world data are often *not* normal. Sometimes it is useful to "straighten" or normalize the data so that a certain statistical method can be used. Table 3.7-3 gives several common data transformations and guidance on when to use them. The lognormal distribution is very commonly found in emission inventories as discussed above (an example is given in the following section); the lognormal transformation is a method that is often used on right-skewed data to create a more normally distributed variable. A transformation might be used if the intention is to use the data for further statistical analysis; such as regression modeling. However, transformation back to the original data should be undertaken with caution, and is not always appropriate. For example, the arithmetic mean of a log-transformed variable can be back-transformed (by exponentiating), but this new value is the geometric mean. For lognormally distributed data, the geometric mean is always less than the arithmetic mean (of the untransformed data). The geometric mean is often used to estimate the lognormal mean and the median, but it is a biased estimate of both (Gilbert, 1987).

The arcsine transform is used when the data are proportions. Examples of these data are also common in inventories. The relative contribution of sources to total emissions, DARS scores (see Chapter 4), or control efficiencies are all expressed as values between 0 and 1.0. If an inventory analyst wanted to know if there were differences in the relative contributions of area sources between two counties (expressed as a fraction of total emissions), for example, a t-test could be used after applying an arcsine transformation to the data. The mean and standard deviations of the raw (untransformed data) should be reported along with the results of the statistical test.

Finally, the square root transform is useful for data that follows a Poisson distribution. This type of distribution often occurs when the data are counts of independent items or events occurring in space or time. Typically, values of zero are common. This distribution is most likely to be encountered when collecting certain types of data that are used to develop factors or activity data. For example, to temporally allocate mobile source emissions, a field study to collect traffic counts might be implemented. The data are collected in discrete intervals, depending on the location, time of day, and length of interval. Some of the values may be zero while others are quite high. These data are likely to fit a Poisson distribution.

TABLE 3.7-2

PROBABILITY DISTRIBUTIONS RELEVANT TO EMISSIONS INVENTORIES

Distribution	Sample Mean	Sample Variance	Examples

Binomial	np, where
	n = number in
	    sample or
	    population,
	p = proportion
		np(1-p)	Proportion of facilities in a SIC group belonging to emissions source category.
			
			Rule penetration (i.e., proportion of area source affected by a rule).

Lognormal	If the distribution is not highly skewed, simplest approach is to use equations shown for normal distribution[a]		See text.
Normal			Rarely found in environmental data but most standard statistical formulas assume normal distribution.
Uniform			Often used as default distribution when true distribution unknown.

[a]For a more detailed discussion of the methods used for estimating the mean, standard deviation and median of lognormally distributed data, see Gilbert (1987).

TABLE 3.7-3

DATA TRANSFORMATIONS USED TO "NORMALIZE" DATA

Transform name	Calculation of transformed data	Use when:
log[a]	$\chi' = \ln(\chi)$	Raw data approximate or are known to follow lognormal distribution.
arcsine (or angular)	$\theta = \arcsin \sqrt{p}$, where p is a proportion	Raw data are proportions between 0 and 1.0; if most data points fall between 0.3 and 0.7, this transformation generally not needed.
square root[a]	$\chi' = \sqrt{\chi}$	Raw data are counts of discrete events (distribution is Poisson, i.e., variance increases with the mean).

[a]If any of original data are zero, a very small number is generally added to all of the original χ values before transformation.

For more discussion of the proper use of data transformations, see Sokal and Rohlf (1969). An example of the use of normality tests and data transformation is given next.

7.2.1 TESTING FOR NORMALITY

The first step is to generate basic statistical summaries of the data. These summaries include the minimum, maximum, mean, median, quartiles, and standard deviation of the data. For normally distributed data, the mean and median should be equal and the minimum and maximum values should be equally spaced below and above the mean. Most likely, this simple test will indicate significant departure from normality. For example, emissions data tend to have a few sources with very high emission rates that produce a highly skewed distribution with a long tail, resulting in the mean being significantly higher than the median.

Table 3.7-4 presents a summary of the basic descriptive statistics for the Los Angeles data set used as an example in the remainder of this section. This data set represents estimated emissions for South Coast Air Basin for the year 2007 for point sources. For each of the pollutants, the descriptive statistics imply a highly skewed distribution. The mean is a factor of 10 greater than the median for all pollutants except for PM_{10}. In fact, the mean is greater

TABLE 3.7-4

DESCRIPTIVE STATISTICS FOR LOS ANGELES POINT SOURCE INVENTORY[a]

Pollutant	Number of Sources	Mean (TPD)	Median (TPD)	Upper Quartile (TPD)	Min (TPD)	Max (TPD)	Standard Deviation (TPD)
TOG	24,432	0.012	0.0025	0.0072	~0.0	3.9	0.067
NO_x	6,980	1.2	0.00088	0.0052	~0.0	380	10
CO	6,004	0.025	0.0011	0.0049	~0.0	10	0.21
SO_2	1,033	3.0	0.00095	0.0090	~0.0	370	22
PM_{10}	8,225	0.0042	0.00052	0.0018	0.0	1.1	0.023

[a]All emissions shown as tons per day (tpd).

than the upper quartile (75th percentile) for all five pollutants.

The second step should be preparation of a histogram of the emissions data. After the initial review of the data presented in Table 3.7-4, it is reasonable to assume that the data must be transformed if some semblance of normality is to be obtained. The most common data transformation is a logarithmic transformation, whereby the emissions estimates are replaced by the natural logarithm (logarithm to the base e) of the emissions data. When this transformations complete, the resultant data many times can be represented by a log-normal distribution.

Figures 3.7-1 and 3.7-2 present two histogram plots of total organic gases (TOG) emissions from the South Coast Air Basin. Figure 3.7-1 gives a histogram of the untransformed emissions data while Figure 3.7-2 presents the data after application of the log transformation. Based upon visual inspection of Figure 3.7-2, the transformation is highly successful in producing a log-normal distribution. The histogram is closely matched by the fitted normal distribution.

Another graphical method for examining the fit of a normal distribution is the expected normal plot. Figure 3.7-3 presents expected normal plots for TOG and NO_x from point sources in Los Angeles. In this plot, the observed emission values (log transformed values for this data set) are plotted on the X axis. On the Y axis, the standardized value of the emissions in plotted. The z value standardizes the distribution to have a mean value of zero and a standard deviation of 1.0. The z value is standard statistical transformation and is computed as follows:
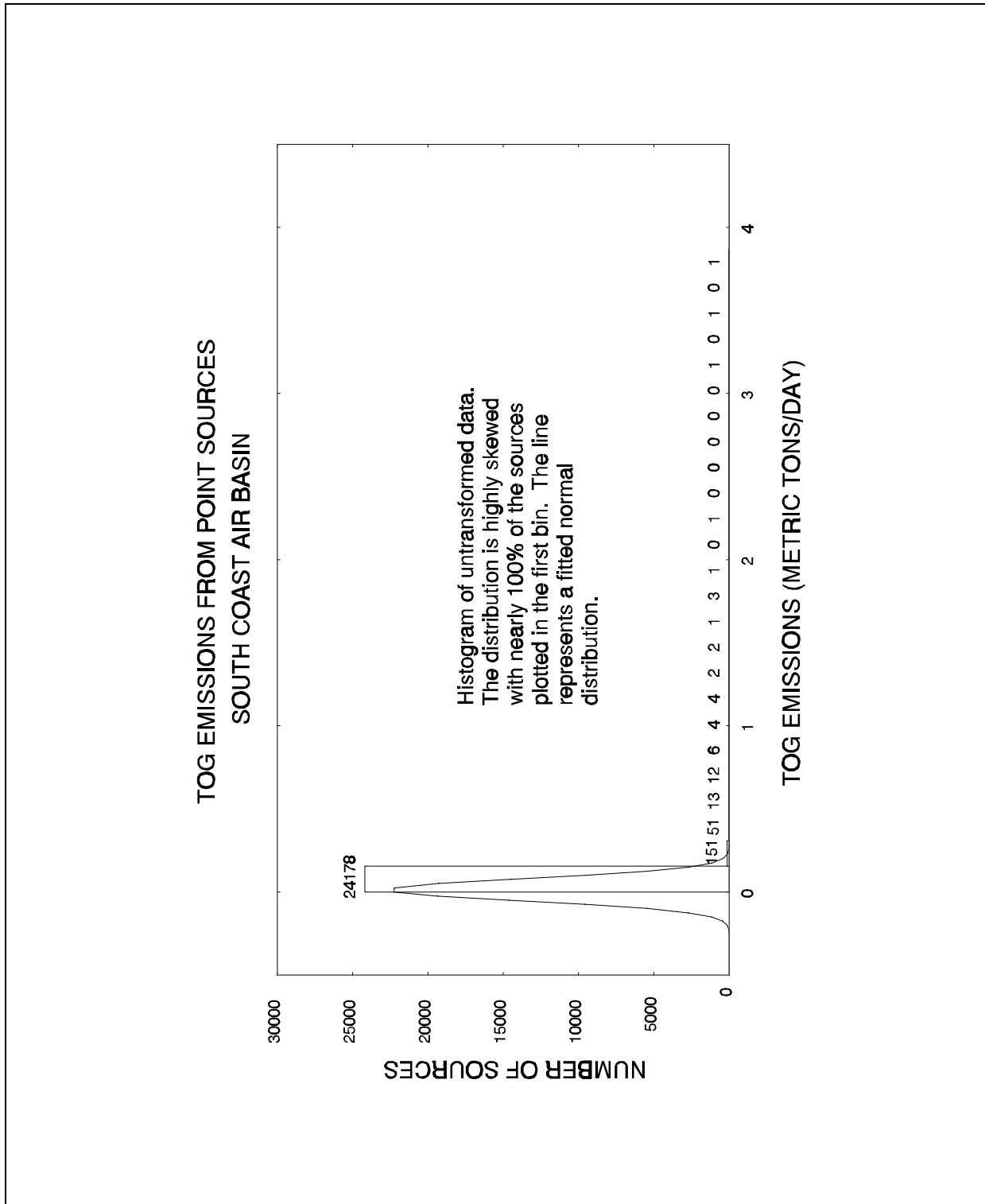
FIGURE 3.7-1. **HISTOGRAM PLOT OF TOG EMISSIONS FOR LOS ANGELES, NO DATA TRANSFORMATION**
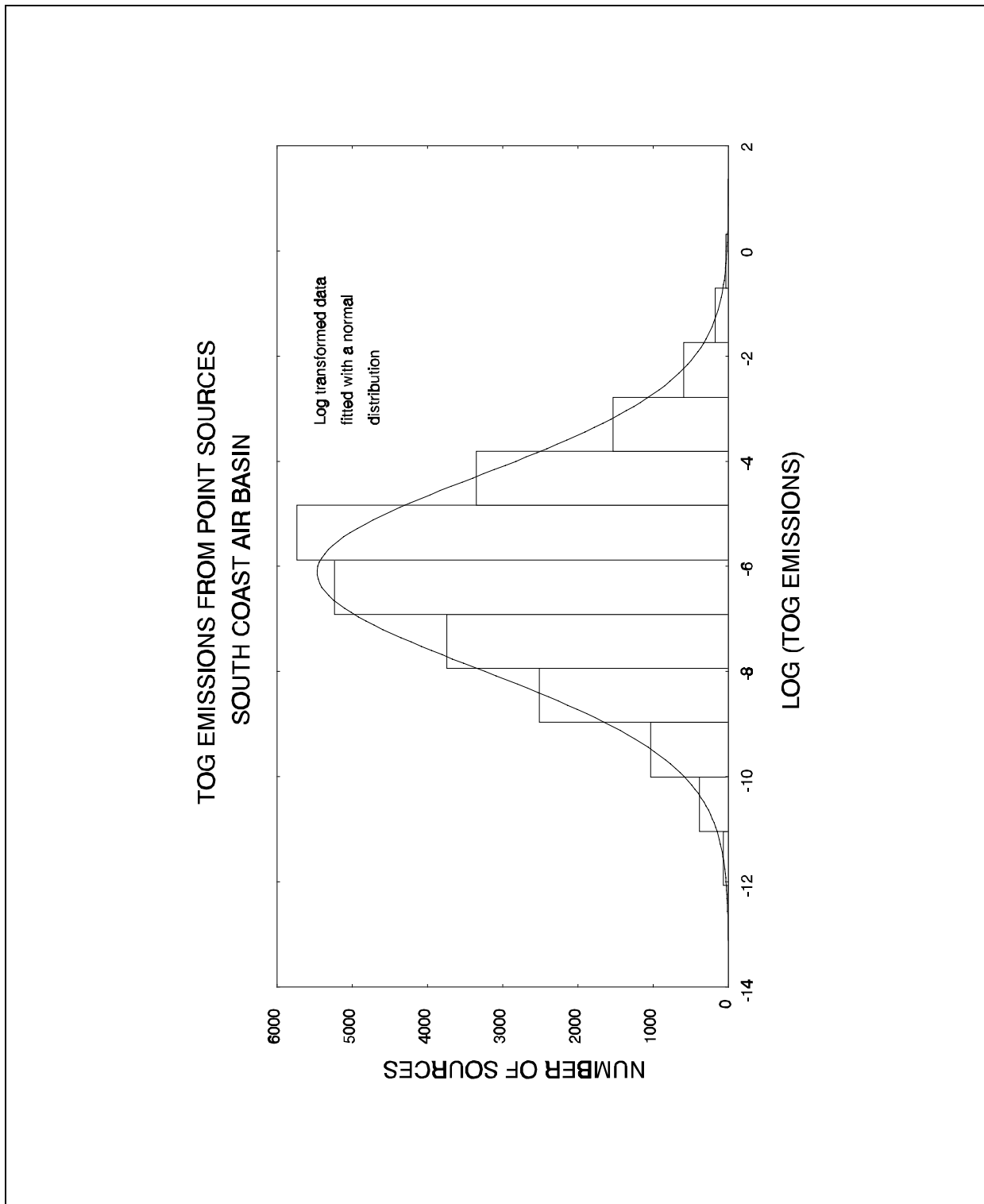
FIGURE 3.7-2. HISTOGRAM OF TOG EMISSIONS FROM LOS ANGELES POINT SOURCES, LOG TRANSFORMATION

EXAMPLE NORMAL PROBABILITY PLOTS OF EMISSIONS DATA
SOUTH COAST AIR BASIN POINT SOURCE EMISSIONS

The points plotting as a
straight line indicate the
data are well fit by a normal
distribution.

95% of the points
will fall within
±2 standard
deviations

Deviation from a straight
line indicates a poor fit
by a normal distribution.

The variable x, sorted from
low to high, is plotted on the
X axis. For a log transformed
variable, $LOG_e(x)$ is plotted.

The extreme values
are not as well fit
as the more central
values.

standard z score of the
ble x is plotted on the Y axis:
x - mean)/standard deviation.
standardized z value is the
ber of standard deviations the
ble x is from the mean.
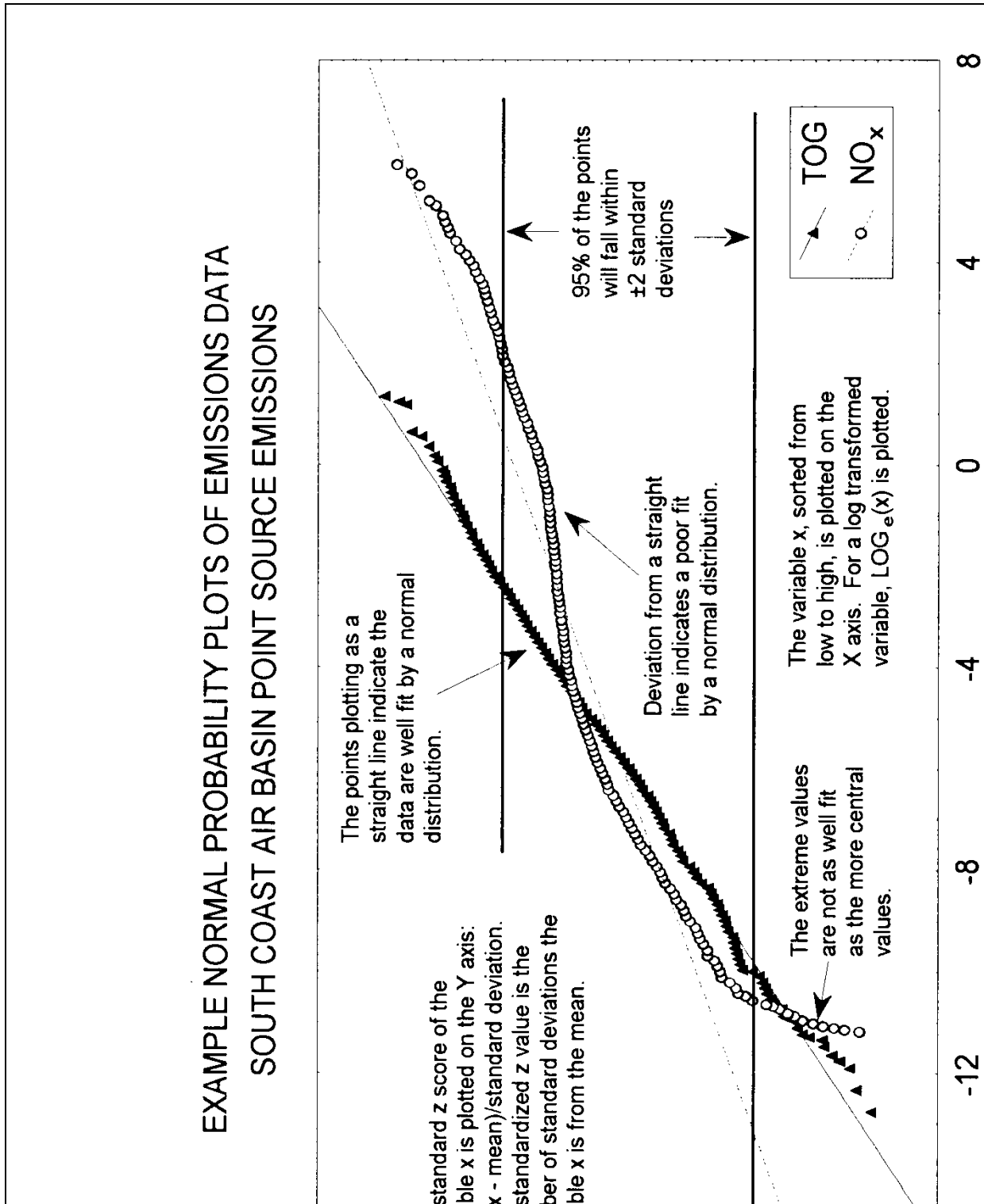
TOG

NO$_x$

-12   -8   -4   0   4   8

**FIGURE 3.7-3. EXAMPLE EXPECTED NORMAL PLOT FOR LOS ANGELES POINT
SOURCE EMISSIONS**

$$z = \frac{\left(x - \overline{x}\right)}{\sigma_s}$$

where:

      z = standard score;

      x = emission value;

      $\overline{x}$ = sample mean; and

      σ_s = sample standard deviation.

For the purposes of the expected normal plot, the distribution being tested is assumed to follow a normal distribution and thus $\overline{x}$ and σ_s estimated from the data set are assumed to be unbiased estimates. For a non-normal distribution, this assumption is violated but the plot itself will identify the lack of fit of the normal distribution.

When the standard score is plotted against the respective value on a linear plot, data from a normal distribution will plot as a straight line on an expected normal plot. As can be seen from Figure 3.7-3, the TOG data for Los Angeles plots as a relatively straight line over most of its range. By comparison, there is a significant deviation from a straight line (and hence log-normality) for the NO_x emissions.

Included on Figure 3.7-3 are elements of the plot that provide insight as to the normality or non-normality of the plotted data. First, if the data are normal, approximately 95 percent will fall within ±2 standard deviations of the mean (between -2 and +2 on the Y axis). From inspection, the TOG data follows a straight line between ±3 standard deviations (approximately 99.7 percent of the data). Both the NO_x and TOG distribution deviate from the straight line at both extremes. This is a common occurrence because the hardest portions of a distribution to fit are the two extremes. For the purposes of emissions uncertainty, the most important factor is the semblance of normality for the bulk of the data. Thus, deviation from normality at the very extremes of the distribution are generally unavoidable but expected.

It is obvious from an expected normal plot when the data clearly do not approximate a normal distribution. Figure 3.7-4 presents an expected normal plot of untransformed Los Angeles point source NO_x emissions. The observed "angle" in the data is very characteristic of a data set that is highly skewed and in need of a logarithmic transformation.

One factor that leads to non-normality in emissions data is illustrated in Figure 3.7-5. This figure presents a histogram of log-transformed NO_x emissions in Los Angeles that demonstrates a bimodal distribution of emissions. Bimodal distributions are common where there are significant differences in the types of sources producing emissions. For NO_x emissions, small industrial boilers and large utility boilers can potentially contribute to the
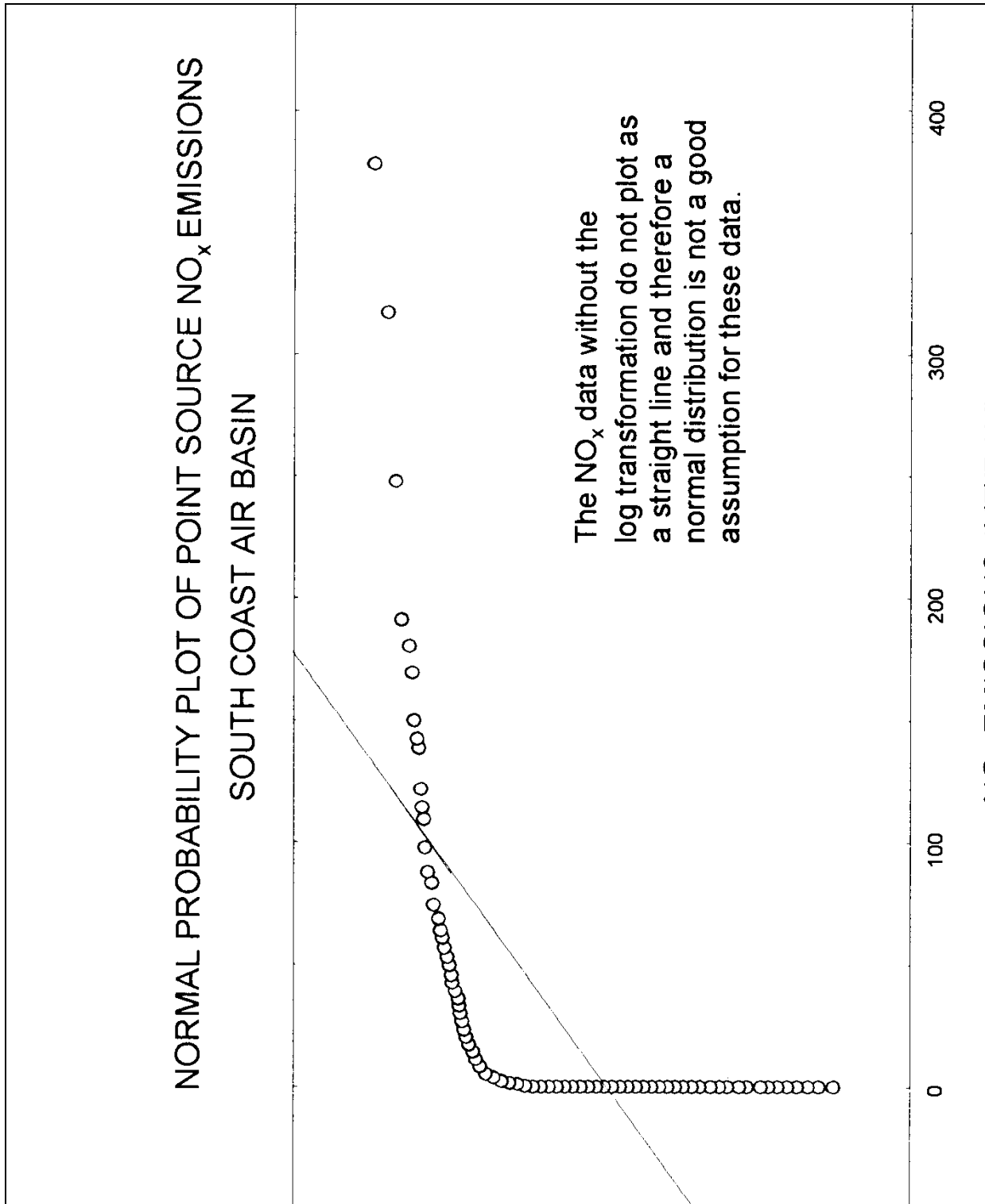
FIGURE 3.7-4. **EXPECTED NORMAL PLOT OF LOS ANGELES POINT SOURCE NO$_X$ EMISSIONS WITHOUT A LOG TRANSFORMATION**
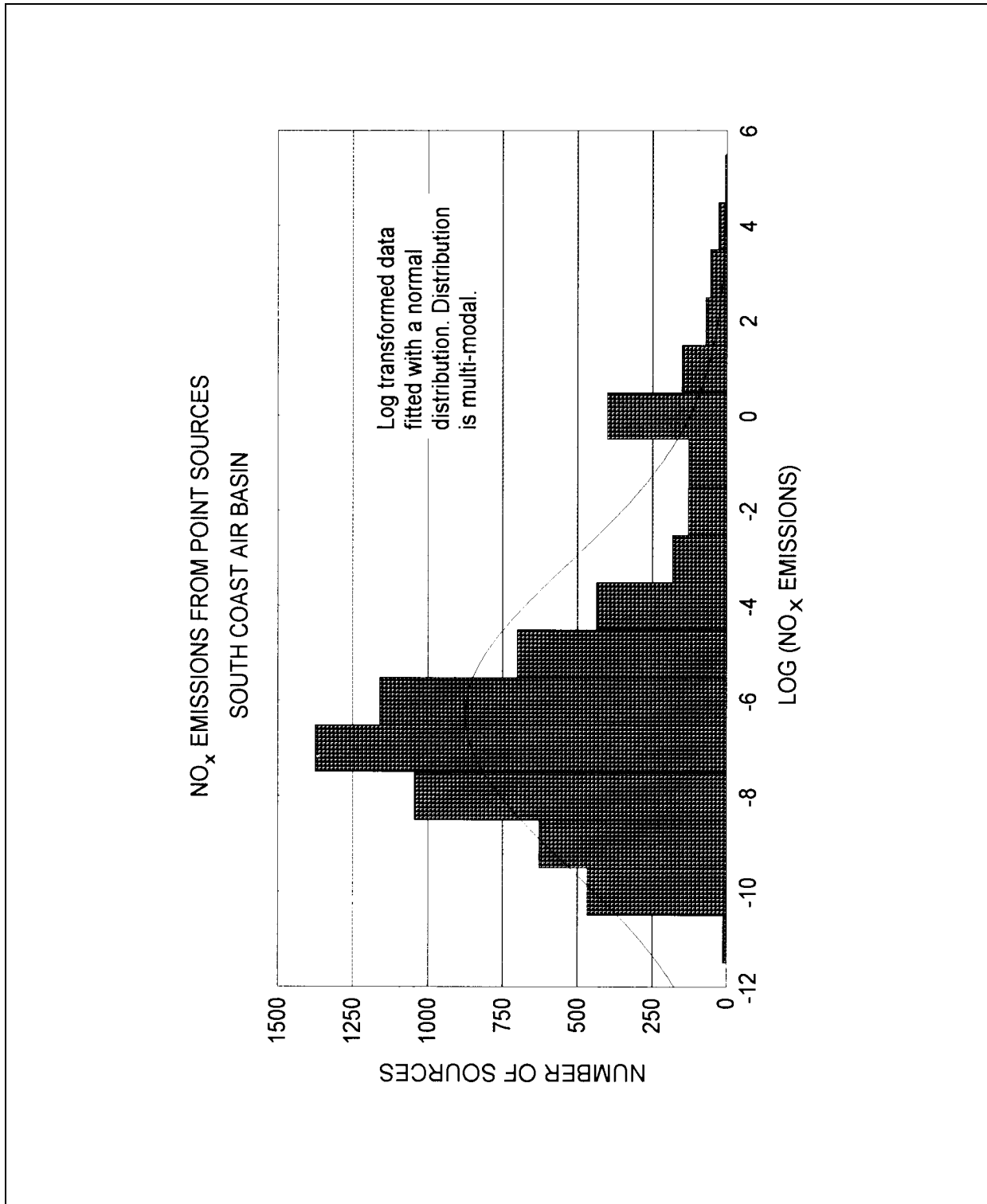
FIGURE 3.7-5. HISTOGRAM OF LOS ANGELES LOG-TRANSFORMED NO$_X$ EMISSIONS DATA ILLUSTRATING A BIMODAL DISTRIBUTION

bimodal nature of NO_x.

Most statistical packages include tests for determining the normality of data. However, care should be taken when judging normality of emissions data on the basis of standard statistical tests such as the Shapiro-Wilk normality test (Shapiro and Wilk, 1965). Emission data sets such as the Los Angeles set used here are very large (over 24,000 sources of TOG in the point source inventory). Because of the large sample size, very small deviations from normality in the distribution are judged to be statistically significant. The above transformed TOG data set, which appears to have a very good visual log-normal fit, fails the Shapiro-Wilk normality test because of the very large sample size. However, for most emissions analysis purposes, the strict deviation of the transformed data set from normality is not important.

7.3 STATISTICAL QUALITY CONTROL

Statistical quality control is a proactive set of procedures in which the assignable causes of variation have been removed from the process (or at least that is the intention) and only random causes are present. The expected error associated with those random causes of variation is characterized by a probability distribution. A tool is then developed based on this probability distribution that can be used to monitor the occurrence of an assignable (and presumably correctable) cause (Woodall and Adams, 1990). This tool may focus on *attributes* or on *variables*. Data that arise from the classification of items into categories are attributes. They are generally measured as counts (or proportions) of the number of items in a given category. For example, in an inventory the QC tool could focus on data entry errors that occur because of incorrect keying of data; the attribute would be a simple "correct/incorrect." When the data are actual measurements, estimates, or calculations, the quality tool is based on variables. If variables are used, the process might be directed towards the value of input data such as stack heights, emission rates, or the emissions themselves.

The type of tool used for statistical quality control is generally some type of control chart or acceptance sampling. The control chart is probably more suitable for continuous processes (although data entry errors for large databases could be monitored using control charts). The concept of acceptance sampling, however, is very similar to the range check concept that is commonly employed for database QC. The difference is that statistical quality control goes well beyond what is normally done for inventory range checks in that a target quality level is specified, a statistically valid sampling plan for the data set is specified in advance, and procedures for dealing with errors are established ahead of time.

7.3.1 AN EXAMPLE OF ACCEPTANCE SAMPLING BY ATTRIBUTES

One of the most common QC activities involves verification that data keyed into a computer database are correct. A state inventory can be very large so that 100 percent inspection (i.e., checking the data to verify correctness) is impractical. The solution is to sample the database, and only check a specified percentage of the data; however, determining the sample design and sample size is not always straightforward. Generally, a stratified random sample is recommended.

The first step in designing a statistical random sample is to divide the data into subcategories. A point source inventory, for example, may be divided into general data (company name, address, owner's name, etc.), location data (UTM coordinates, county, etc.), stack data, process data, or other categories. The importance of these categories will vary. Errors in the general data may be of minor consequence, process data may be critical. The agency should prioritize the data categories as to importance. Sample sizes will depend partly on the importance of the category.

The next step is to choose the acceptable level of error. Several statistical QC symbols and their meaning are defined below (derived from Grant and Leavenworth, 1988):

N	=	number of items in a given lot or batch.
n	=	number of items in a sample.
D	=	number of incorrect items (i.e., data elements not conforming to specifications) in a given database of size N.
r	=	number of incorrect items (i.e., data elements not conforming to specifications) in a given sample of size n.
c	=	acceptance number, the maximum allowable number of incorrect items in a sample of size n.
p	=	fraction incorrect. In a given database, this is D/N; in a given sample, it is r/n.

In general, the inventory preparers will want to minimize the number of errors, so c=0. That is, if any incorrect data elements are found in the batch that is inspected, the data set is unacceptable. In practice, this means that either: (1) the entire data set is inspected and incorrect values are corrected, or (2) the errors in the sample are corrected and the sampling/corrected process is repeated until no errors are found in a sample. The second approach may still allow some errors to remain, but it is much more cost-effective for very large data sets.

Figure 3.7-6 shows the probability that no errors will be found (i.e., P_a or the probability of acceptance) for a given sample size (n) from a database of size N = 5,000. The actual number of incorrect data (D) in the database is shown on the X axis. The graph shows that if 100 points are sampled (n=100) from this data set, there is a 5 percent ($P_a = 0.05$) chance of finding no errors when the true error rate is about 160/5,000 or 3.2 percent (p = 0.032). A larger sample size decreases the probability of accepting a defective data set. For example, if n = 500, the probability of accepting a dataset with p = 0.032 is near zero. Note that this example assumes only one sample will be taken. Better quality can be attained if the database is repeatedly sampled, inspected, and corrected until the desired level of quality is attained (discussed further in the next section).

7.3.2 SPECIFYING A SAMPLE PLAN

Inventory QA plans often specify a percentage of data elements to be sampled, incorrectly assuming that the ratio of sample size to data set size is important. Figure 3.7-7 shows the fallacy of this idea. The curves show that from a quality control perspective the absolute size of the sample is more important than its size relative to that of the data set. Figure 3.7-7 shows four curves for a sampling plan that specifies 10 percent of the inventory be checked. Note that for a given percent incorrect, the smaller N is, the less protection is afforded by using a 10 percent sampling scheme. For example, with only 2 percent incorrect, the probability of accepting the data set of N=1,000 using the 10 percent sampling scheme is around 0.12. The risk of accepting a "bad" dataset is even higher for smaller data sets. This suggests that setting a threshold sample size may be a better strategy. For example, the sample design could specify inspection of data elements for all sources above a certain size, and then sampling a percentage of the remainder. Or, the sample size could be preset at 500 where N≥500, and 100 percent sampling if N<500.

The sampling plan design should also specify the criteria for determining an adequate number of samples. This can be done *a priori* by specifying the exact number of samples. Or, an iterative approach can be used which requires meeting a target level of quality (or maximum error rate that will be acceptable). For example, the error rate found in one sample may be used to estimate the overall error rate (the average outgoing quality or AOQ) as follows:

$$AOQ = 100p * P_a$$

where P_a is the probability of acceptance as shown in Figures 3.7-6 and 3.7-7, and p = r/n. For example, if p = 0.04 and $P_a = 0.012$, the AOQ = 0.048. This says that the estimated error rate in the database is 4.8 percent (or, 4.8 percent of the data elements are likely to be incorrect). For a more detailed discussion of AOQ and the theory behind it, see Grant and Leavenworth, 1988.
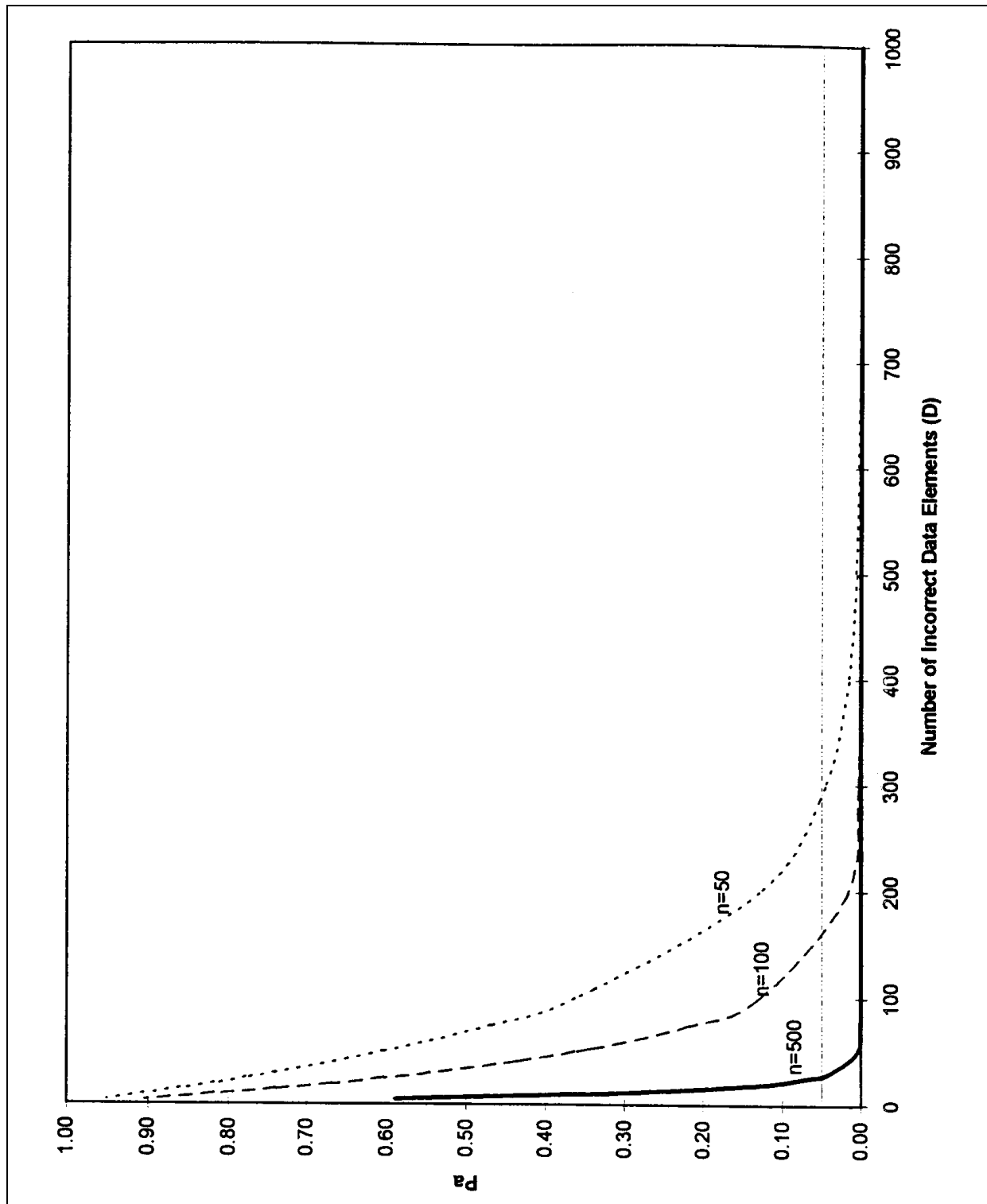
FIGURE 3.7-6. PROBABILITY OF ACCEPTING A DATASET AS ERROR FREE FOR THREE DIFFERENT SAMPLE SIZES

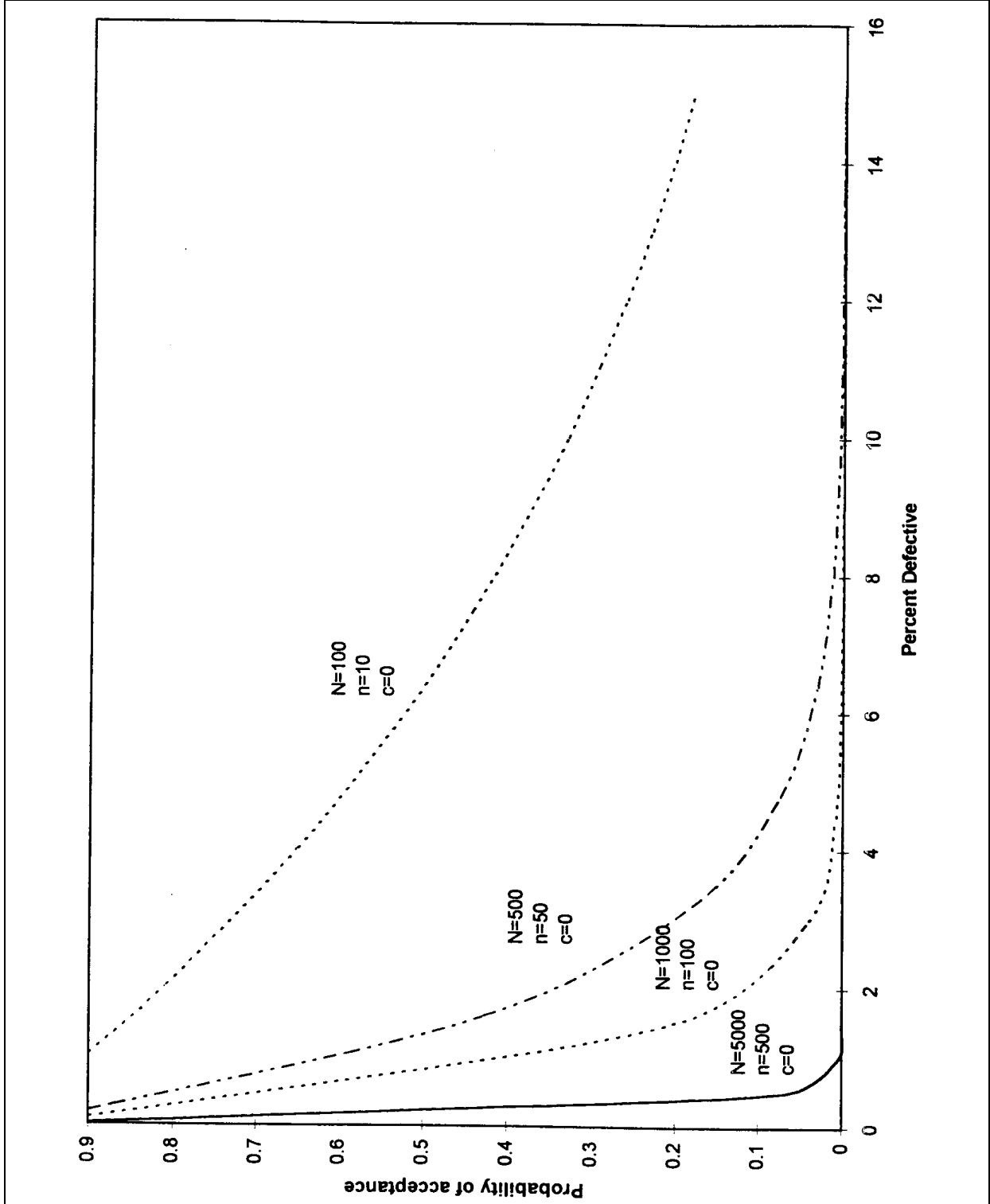**FIGURE 3.7-7.** PROBABILITY OF ACCEPTING A DATASET AS ERROR FREE WHEN 10% SAMPLE SIZE IS USED

If the AOQ is too high, another sample may be chosen. Again, any errors found are corrected, and p, P_a, and AOQ are calculated. This process is repeated until the AOQ reaches an acceptable level. Note that this assumes sampling with replacement; that is, each sample is randomly chosen from the entire data set and may include items previously sampled. An alternative approach is to not include previously sampled data elements in subsequent samples (i.e., sampling without replacement). If this approach is used, AOQ is calculated by adjusting for the previously checked and corrected data as shown:

$$AOQ = (100\text{-}f)p * P_a$$

where f = percent inspected and corrected.

The QA program plan should specify the desired AOQs and sample size (n) for each subset of the data. The procedures for sampling should be described in as much detail as possible. Calculation of P_a and AOQ values can be easily performed using the SAS QC$^®$ function PROBHYPR; other statistical QC packages are also available that can calculate these terms.

7.3.3 OUTLIER ANALYSIS: ACCEPTANCE SAMPLING BY VARIABLES

Statistically based outlier analysis can be used to check the ranges of specific data and flag values that appear to be in error. This use of statistics to flag outliers is similar to the concept of acceptance sampling by variables used in statistical quality control programs. A common approach is to use the mean and two (2sd) or three (3sd) standard deviations as the basis for the acceptable range. Although three standard deviations is generally used to screen data sets and reject extreme values, for the purposes of inventory QC, two standard deviations may be more appropriate. A large proportion of the data flagged using the 2sd test is likely to be correct, but use of the 3sd test will probably not detect any errors except the very extreme ones.

It is important that the expected distribution of the variable being checked is considered when setting the acceptance criteria (see discussion above under "Descriptive Statistics"). If the underlying distribution is highly skewed to the right (e.g., lognormal), using the arithmetic mean and standard deviation may not be appropriate. In fact, a random sample from a lognormal distribution will tend to result in a large standard deviation, often exceeding the mean. Adding 2sd or even 3sd to the mean may still fall short of the possible range of values at the high end; subtracting 2sd may result in a negative number. Thus, the range check will not detect any values too small (assuming the real data set is always positive), and will flag too many "errors" at the high end.

Four different methods can be used to deal with this problem. The first is simply not to rely on statistical procedures for range checks. Engineering judgment can be used to set an

appropriate upper and lower bound for each variable. This method will work reasonably well assuming that all the variables in the data set are sufficiently understood, and that the "true" range and distribution of the data do not change appreciably between years or geographic regions.

The second approach is to calculate the mean or other statistics using the method that is appropriate for the specific distribution. The greatest advantage of this approach is that it is more likely that errors will be detected, and it reduces the likelihood that correct values will be flagged. The problem with this method is that it requires more information and work to set up the appropriate criteria; it also assumes that the correct underlying distribution can be identified which is often not the case.

The third approach is to use the arithmetic mean and standard deviation of the transformed (and normalized) data. For example, the natural log of the data may more closely follow a normal distribution. If this method is used, the transformed data should be tested using a test for normality to determine if the transformation has had the desired effect. Data must be transformed back to their original form after the analysis is complete (Table 3.7-3 gave examples of transformations).

Assuming that the data are reasonably normal, the outlier test may be made with or without reference to a pre-determined "correct" value. An example of the latter was given in the first paragraph of this section. If the data are normally distributed, 68 percent of the data will fall within 1sd of the mean; 95 percent, 2sd; and 99 percent, 3sd. If more than 1 percent of the data are greater than 3sd away from the mean, these data are suspect.

Of course, the data may be internally consistent (and normally distributed) but still incorrect. Comparison to a reference value should be used as a check. The reference value may be based on a different data set; for example, the distribution of stack heights may be taken from a national inventory and used as the reference distribution for a county- or state-level dataset. Or, the reference value may be based on previous inventories in the region, or based on engineering judgment. Typically, the mean value of the variable is compared to an expected mean using a t-test.

The t-statistic is calculated as:

$$t = \frac{\overline{x} - \mu}{s/\sqrt{n}}$$

where:

$\quad$ t $\quad$ = $\quad$ the calculated test statistic;

$\overline{x}$	=	the mean of the test data set;
μ	=	the preestablished mean (or reference value);
s	=	the test data set standard deviation; and
n	=	the number of data values used to calculate the test data set mean and standard deviation.

Assuming that the data are normally distributed, the distribution of the test statistic follows the *Student's t distribution*. The t value can be compared to a statistical table of values generated for the Student's t distribution for various sample sizes and levels of significance. The various sample sizes within a Student's t distribution table are referred to as the *degrees of freedom*. The number of degrees of freedom is equal to the sample size (in this case, the number of values in the data set) minus one. If the absolute value of the test statistic is greater than the value in the Student's t distribution table for a specified level of significance and degrees of freedom, the conclusion would be that the calculated average value is significantly different than the number entered into the average value field. If this is the case, the data must be examined in greater detail to determine if the data are in error, or if the preestablished value entered into the average value field should be changed.

The fourth approach is to use nonparametric methods to evaluate the data. Nonparametric methods make no assumptions regarding the distribution of the data; the sample median, rather than the mean, is used as the basis for testing. A *sign test* can be used to test whether the median of the data is significantly different than a preestablished median. The preestablished median is first subtracted from the values of every data point in the sample, and the total number of positive values (a) and negative values (b) are recorded. Any zero differences are omitted from the test. The test statistic is:

$$\chi^2 = \frac{(|a - b| - 1)^2}{n}$$

where:

χ^2	=	the test statistic;
a	=	the total number of positive values;
b	=	the total number of negative values; and
n	=	a + b.

The test statistic follows a *Chi-square distribution* with one degree of freedom. The value of the test statistic can be compared to a table of values for the Chi-square distribution at various significance levels. If the test statistic is larger than the tabular value, the conclusion is that the sample median is significantly different from the preestablished median.

If the total number of positive and negative differences is larger than 25, a normal approximation to the binomial distribution must be used:

$$Z = \frac{a - 0.5n}{0.5\sqrt{n}}$$

This test statistic (Z) can be compared with the value in a normal distribution table for a selected level of significance.

7.4 STATISTICAL PROCEDURES FOR COMPARABILITY ANALYSIS

Summary statistics are most useful for comparing inventories. Although statistical measures are often used as the basis for comparisons, any decisions made or conclusions drawn from these statistics are usually subjective. That is, the reviewer will compare means, plot emissions versus a variable thought to be correlated with emissions, or evaluate correlations between variables. The reviewer then decides (using his or her own unwritten criteria) that the data are "different" or "reasonably similar." No published references were found that indicate hypothesis testing has been used to determine if two data sets (or inventories) are significantly different, although this method may be appropriate for certain types of analyses.

The types of comparisons most commonly used include:

- Comparisons between inventories;

    -- between years (same region)
    -- between regions (same year)

- Comparisons to a reference distribution;

    -- between a region and a larger geographic area (such as state to national)

- Comparisons of emissions to a surrogate with an expected predicted relationship (e.g., plot of on-road emissions vs. VMT).

All of the above are useful for the evaluation of inventories; however, their uses strictly for QA/QC need to be considered very carefully. As with other forms of reality checks, differences between two statistical measures do not necessarily mean an error has occurred; similarly, errors will not always be obvious when using this method.

In most cases, an informal comparison of the statistics is sufficient. Often the differences are so obvious as to need to no further statistical analysis; emissions from one inventory may be

consistently higher or lower than the other (i.e., biased) and the reasons are easily traced to differences in methods or assumptions used. Biases in inventory data may occur if different methods, factors, activity data, or assumptions are used; within a state (or region), consistent approaches will minimize the occurrence of this type of bias (see Chapter 2, *Planning and Documentation*). However, if inventories prepared by different people and/or for different geographic entities are compared, consistency in approaches cannot be assumed (and is not very likely).

Differences between inventories cannot be assumed to be the result of errors; for example, suppose that evaporative emissions from gasoline marketing are consistently higher (when expressed on a per gallon basis) in two inventories. The QA reviewer should first determine if there is a reasonable explanation for the apparent bias. One state may have implemented Stage I and/or Stage II controls resulting in lower emissions. It is best when conducting a statistical comparison for QA purposes to first remove all the assignable causes of variation. For example, comparisons of uncontrolled emissions might be a better way of detecting possible errors for the gasoline marketing example. Any differences in emissions are more likely to be due to inconsistences or errors in the underlying calculations.

When visual inspections do not reveal any obvious differences, it is generally harder to conclude that the data are correct. Most inventory analysts feel that the uncertainty of emission estimates is too high to allow conclusions to be drawn when small differences between emissions are seen. In this case, the use of statistical tests to detect differences can be of use. The t-test or sign test described in the previous section can be used to determine if there are statistical differences between inventory data if two data sets are being compared. If more than two data sets are being tested, an analysis of variance (ANOVA) can be used for normally-distributed data, or the nonparametric Kruskal-Wallis test should be used if assumptions of normality can be met.

7.5 EXAMPLE OF A STATISTICALLY BASED COMPARABILITY ANALYSIS: REGRESSION MODEL USING DUMMY VARIABLES

When preparing an inventory, it is sometimes necessary to evaluate data prepared by another expert or agency. A common example is found in the development of onroad mobile source emissions; VMT estimates are often done by experts outside the agency preparing the inventory. In this example from North Carolina, the state's department of transportation (DOT) supplied a database of VMT by county over an eight-year period. The inventory analyst at the NC DEHNR had several objectives for this analysis: (1) assess the reasonableness of the estimates, (2) check for any errors in the data, and (3) develop a model to be used for projections of VMT in the future. The method used was to develop a regression model using dummy variables. Dummy variables, sometimes called zero-one variables, have a value of one when the characteristic being described is present in an observation or is set equal to zero otherwise.

Seven North Carolina counties, within three ozone maintenance areas, were chosen for this analysis to illustrate one method that may be used to separate the distinctive intercept and slopes associated with reported VMT. A dummy variable was constructed for each county which has the effect of shifting the intercept term. In addition, groups of counties in the TRIANGLE (Durham and Wake), or the TRIAD (Davidson, Forsyth and Guilford) were coded to distinguish those observations from the remaining base group around CHARLOTTE (Gaston and Mecklenburg). These TRIANGLE and TRIAD dummy variables were then multiplied by the trend variable TIME to create a slope shifting effect between these areas.

The basic method for projecting VMT involves linear trend extrapolation using each separate county VMT over the eight year period. Visually checking this combined data for possible errors would be difficult, but there may be advantages to looking at all the counties together or "pooled," for the purpose of comparing growth rates between the three specific areas of the state. If the model, as constructed, can account for a large percentage in the variability, then the residual or difference between the reported VMT value and the predicted value from the model can be used to indicate possible errors.

Figure 3.7-8 shows a graph of all reported VMT values versus the predicted values from this model. Visual inspection of the plot revealed a possible keying error from Durham County in 1988 (circled on the figure). The originator of the data set was contacted, and confirmed that this value was incorrect. The value was corrected and the regression was recalculated. This graph can also be used to perform other types of QA checks. For example, the relative ranks and slopes of the county-level data can be compared as a type of reality check (see Section 1). The reviewer might look at the population of each county, the miles of different road types, and other factors that presumably affect VMT to determine if they are consistent with the pattern seen in the data.
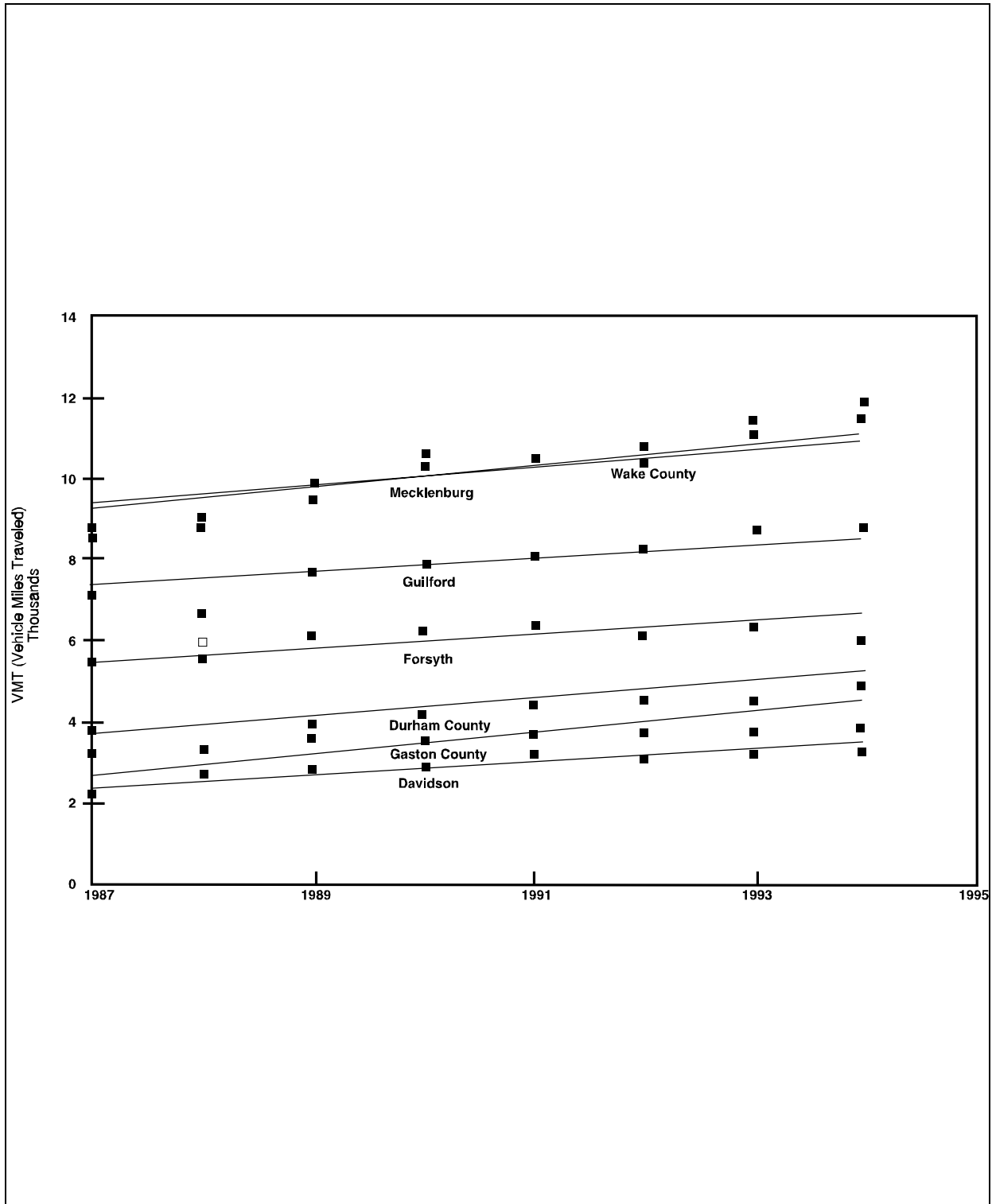
FIGURE 3.7-8. GRAPHICAL COMPARISON OF REPORTED AND PREDICTED VMT VALUES

TABLE 3.7-5

RESULTS OF DUMMY VARIABLE REGRESSION ANALYSIS OF COUNTY VMT DATA

X Variable Name	X Coefficient(s)	Standard Error of Coefficient	"t" Statistic
Time	273.3	52.54	5.20
Davidson	2388.6	277.00	10.52
Durham	3839.8	250.60	15.32
Forsyth	5710.5	227.00	25.16
Gaston	2744.9	250.60	10.95
Guilford	7683.4	227.00	33.85
Mecklenburg	9677.4	250.60	38.62
Wake	9772.8	250.60	39.00
Time*Triad	-100.1	67.83	-1.48
Time*Triangle	-38.2	74.30	-0.51

The regression results can be interpreted around the base case of what is occurring in the Charlotte area. The t-statistic (shown in Table 3.7-5) can be used to determine the significance of including each trend or dummy variable in the model. A general rule for evaluating the t-test is that an absolute value greater than two is significant at the 0.95 confidence level. The model suppresses the normal calculation of an intercept term by assigning each intercept a shifting county dummy variable. These were all highly significant, which indicates that the initial VMT levels between counties are different. The CHARLOTTE area growth trend variable coefficient (time) of 273.3 equals the VMT increases each year and was quite significant for the base case. The slope shift trend for the TRIAD was -100.1, which means that for those three counties the annual growth in VMT was only 173.2, with a t-test value of -1.48 indicating a mildly significant shift. In comparison, the slope shift value of -38.2 for the TRIANGLE counties had a low t-statistic value of only -0.51. This result may be interpreted to mean that while the annual growth of 235.1 in VMT for the TRIANGLE is smaller than the Charlotte area, it should not be considered as significantly different.

This type of analysis may be used by the inventory developer and cited as the basis for any assumptions subsequently used to develop the inventory. For example, the inventory developer may argue that one growth factor can be applied to all counties except those in the TRIAD, and cite this analysis as the basis for that assertion. Alternatively, the peer reviewer (or technical auditor) may perform this type of analysis to test the validity of an assumption used to develop an inventory. If, for example, the project inventory had been prepared using one growth factor for all counties, the peer reviewer might challenge that based on these results.

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8

INDEPENDENT AUDITS

QUICK REVIEW

Definition:	A systematic evaluation to determine the quality of a function or activity.
Objective:	Ensure that adequate quality control measures are planned and implemented to help develop a complete and accurate inventory.
Optimal usage:	At critical steps in the inventory development process that could affect the accuracy and completeness of the emissions data.
Minimum expertise required:	Moderate to high technical and auditing experience. Auditors should have audit experience and be able to comprehend the technical process and assess whether approved procedures are followed. An audit team of technical and quality professionals may be required for more complicated inventories.
Advantages:	(1) Help provide confidence in the accuracy and completeness of the emissions results, (2) provide an objective assessment of the effectiveness of the quality control (QC) measures implemented by the emissions inventory development team, and (3) foster continuous improvement in the inventory development process.
Limitations:	(1) Additional staff and funds may be needed to conduct independent audits, and (2) may add to the time required to complete the inventory.

8.1 OVERVIEW OF METHOD

Audits are managerial tools used to evaluate how effectively the emission inventory team complies with predetermined specifications for developing an accurate and complete inventory. As discussed in Chapter 1 of this volume, the EIIP's mission is to develop guidance to improve the emission inventory development process. The development of quality programs, as discussed in Chapter 2, is encouraged to establish effective procedures and standards to increase data quality. After implementing these procedures, audits are conducted to determine whether the procedures are effective and whether additional QC is needed to improve the (procedures and hopefully cut the costs associated with inventory development).

Specifically, audits are managerial tools used to:

- Identify staffing problems, particularly areas where understaffing or inadequately trained staff may adversely affect quality;

- Evaluate the effectiveness of the technical and quality procedures used to develop the emissions data;

- Help ensure the completeness and accuracy of the emissions data;

- Determine whether data quality objectives are being met;

- Determine the need for additional QC measures; and

- Streamline the costs associated with the inventory development activities.

The overall goal of the audit program is continuous improvement in the performance of people, processes, and systems. When continuous improvement becomes a reality, more efficient methods are incorporated, data quality improves, and costs are reduced.

A good audit program is one of the key elements of an effective quality program because it helps to identify the sources of errors and ensures that corrective actions are taken to eliminate them. Because of the importance of the audit to continuous improvement of emissions data, audit planning must be conducted along with the technical plans for inventory development. Quality personnel must be familiar with the critical elements of a good audit program and the types of audits that can be conducted to help meet the data quality objectives established for the emissions data.

The purpose of this section of Chapter 3 is to provide information about:

- The elements of a good audit program;

- The types of audits that can be conducted; and

- Preferred and alternative audit methods that can be implemented.

This information should then be used to design an audit program that ensures the development of continuous improvement in your emissions inventory data.

8.1.1 ADEQUATE TRAINING

Auditors must be adequately trained, have good communication skills, and be able to foster good team relationships with the inventory development team members to develop a successful audit program. They must understand the technical aspects of the work and have auditing experience in order to identify sources of quality concerns and make reasonable recommendations for corrective actions (RCAs). When the technical work is very complex, an audit team of quality professionals and technical experts may be needed. Whatever the make up of the audit team, the members of the audit team must have sufficient training to understand the data and inventory procedures used to estimate emissions.

In order to intelligently discuss the inventory procedures, evaluate the appropriateness of the procedures, and develop a written document that clearly identifies the findings and RCAs, good communication skills as well as technical experience are needed. The auditor must be able to objectively identify the deficiencies and communicate the RCAs in a "constructive" manner, while maintaining good team relationships. This is not an easy task, but it should always be the auditor's goal. If good team relationships are not built, communication of concerns that arise during the development of the emissions data are often not shared with the auditors and a true picture of how well or poorly the work is progressing may never be attained.

The auditor should never be viewed as an inspector who legislates rules and regulations for doing work; instead the auditor must be viewed as an inventory development team member who wants to help save time, improve procedures, communicate the need for additional support and resources to management, as well as improve the effectiveness of the systems and quality of the data. The inventory development team must feel that the goal of the auditor is to "help" rather than "hinder" their efforts to achieve the common goal of developing a complete and accurate inventory.

8.1.2 MANAGERIAL SUPPORT

Without senior managerial support, the audit program is doomed! Who will provide the equipment and people required to do the work? Who will see to it that the actions requested to address the quality concerns found during the audits are taken? Who will approve the audit program?

Before beginning any quality program, senior management must agree that the audit program is needed, support the efforts of the auditor in developing the program, and approve the program prior to its implementation. If these steps are not followed, the auditor will have no recourse if a team member or inventory development manager decides to not act upon the RCAs. Therefore, the auditor works closely with senior management to develop quality procedures and programs that are sufficiently funded and include measures that are agreed upon to be needed to achieve an accurate and complete emissions inventory. The position of senior management (see Ron McKernan) in the organization could be as presented in the example organization chart included as Figure 3.8-1.

8.1.3 GOOD PLANNING

The auditor must adequately plan the audit activities in order for them to be successful. This planning should at least include the following:

- Reviewing the inventory work plan and QAP;

- Reviewing technical procedures that are critical to the technical soundness, completeness, and accuracy of the emissions inventory;

- Identifying the key steps in the inventory development process that will affect its completeness and accuracy;

- Reviewing the results from previous audits (if any);

- Developing an audit checklist that will help to provide a thorough review of applicable systems and data; and

- Developing an audit schedule that includes auditing as many of the critical phases of the inventory development process as possible.

The first documents to review when preparing for the audit are the work plan and QAP. These documents provide the scope of work and identify the technical procedures to be followed. In addition, the QAP describes the approved QA/QC procedures to be used. The QAP is usually developed with the assistance of the auditor to ensure that there is agreement
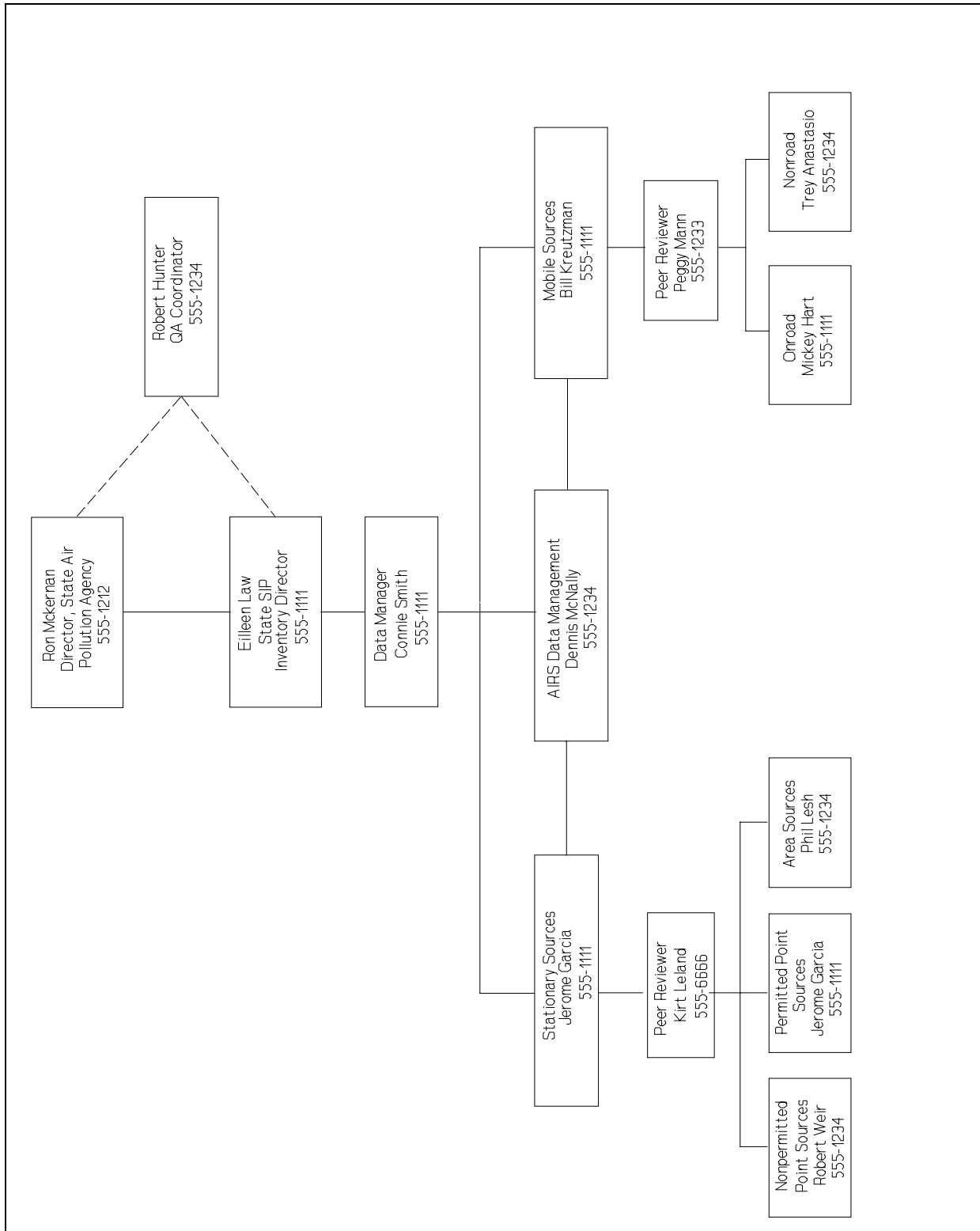
FIGURE 3.8-1. EXAMPLE SIP EMISSION INVENTORY ORGANIZATION CHART

concerning the level of QA/QC required to achieve the technical and data quality objectives.

As a result of previous experience auditing similar inventory development activities, an experienced auditor may help identify steps in the inventory development and reporting processes where additional QA/QC may be helpful. He or she may help define more realistic data quality objectives because trends may have been revealed during previous reviews of historical data. In addition, if data completeness and accuracy were the primary concerns during reviews of previous data, additional QA/QC may be recommended during the development of the data collection, management, and technical review procedures.

During the review of the work plan and QAP, the auditor should answer the questions listed below:

- Were the work plan and QAP approved by the appropriate personnel?

- Were the EPA requirements for developing the work plan and QAP met?

- Are there a sufficient number of experienced personnel to develop the inventory within the agreed upon time frame?

- Are the responsibilities of key personnel identified?

- Will the work be adequately supervised?

- Is the objective of the work clearly stated along with the objectives for data quality?

- Is the technical approach sound?

- Are the procedures for documenting, maintaining, and storing data described?

- Are the federal/state requirements for developing the inventory discussed along with the procedures to be followed to achieve them?

- Are the reporting requirements described?

- Are milestones identified to help meet the deadline established for completing the inventory?

- Is the budget mentioned and is it adequate for the work projected?

     •   Are adequate QA/QC measures described (internal and external)?

Deficiencies found during the review of these documents are documented and brought to the attention of the manager of the inventory development activities as soon as possible.

In addition to the planning documents, the auditor may also review technical standard operating procedures (SOPs) and user's manuals which describe how the data will be gathered, the technical procedures for calculating emissions, and the reporting guidelines (an example is included in Figure 3.8-2). The auditor should look for completeness goals when determining the sources of emissions and a sound technical approach to calculating emissions results. Good SOPs are needed to provide consistency in the approach to gathering data, reviewing it, and developing emissions results. Standard operating procedures are more commonly used in emissions measurement programs; however, written procedures for gathering and using data for emissions inventories are also recommended (see Chapter 2).

The auditor should consider personnel training and supervision of inventory development activities as two of the most important steps in the development of a complete, accurate, and technically sound inventory. Therefore, the organization of the inventory development team and experience of the team members should be reviewed after a basic understanding of the scope of the work and technical expertise required to prepare the inventory is developed.

Adequate training can also be evaluated during the personnel interviews or audits. This evaluation could include the review of personnel training records for evidence of related experience. If deficiencies are found, plans should be made to provide training prior to or during the inventory development process. There should also be evidence of sufficient senior personnel supervision of employees who are less experienced and are being trained to perform inventory development activities.

If previous audits were conducted, the results from these audits are reviewed to determine the quality issues that were identified and actions recommended to eliminate them. The corrective action plan should be a topic of discussion during the audit and, if needed, follow-up activities should be conducted.

After reviewing all of the documents that will help provide a thorough overview of the inventory process, the auditor determines which systems and procedures are key to the successful development of a complete and accurate inventory. These critical procedures and systems will at least include an assessment of the management/supervision of the work, inventory development plans, data gathering activities, completeness checking, data documentation procedures, procedures used to identify emission sources, methods used to calculate emissions, QC measures, and reporting requirements. Questions concerning these critical phases in the inventory development procedures are then included in an audit checklist. Critical phases in the inventory development process may be determined by

KEY ELEMENTS OF DATABASE USE AND OPERATION

1.   The system sets up the required data screens for the type of inventory to be
      developed.

2.   The initials of the operator and the date are attached to each added or updated field.

3.   The desired area or geographical locations can be selected.

4.   For point sources, detailed source information module is used rather than the general
      module to allow the inclusion of small plant VOC emissions values during summary
      calculations on a county or grid level. Emissions for remaining point source
      categories can be added manually.

5.   A calculator is available on line.

6.   The system screens each data field (length, type of characters) prior to accepting the
      data added or edited.

7.   Each field has a help screen or look-up table (SC Codes, SIC Codes, emissions
      estimate methods, pollutants, etc.).

8.   When data are deleted, all the relative data associated with that key field are deleted
      to avoid the existence of orphan data. The data deleted are retained in the systems
      utility area until a request for removal is received. The data held in the utilities part
      of the system are not used for summaries or calculations.

9.   Nonbanked annual emissions, ozone seasonal daily emissions, and carbon monoxide
      daily emissions can be calculated. If the required data are included, carbon monoxide
      seasonal calculations can be adjusted to daily rather than 8 hour periods.

10.   When data are ready for transportation, transaction files are created. Data are edited
      prior to transport. If the required data are not available or in the correct format, error
      codes or messages will be printed to the screen. All corrections must be eliminated
      prior to transport.

11.   The screening or validation conducted during data editing includes 1) checking the
      field length and data type (numeric or alpha-numeric) and 2) comparing entries
      against look-up tables.

FIGURE 3.8-2. KEY ELEMENTS OF DATABASE USE AND OPERATION

examining the example Information Flow Chart, shown in Figure 3.8-3. This chart shows data gathering, information flow, and QC activities for a typical inventory development process. Any place where QC activities are indicated are also appropriate places for QA audits. In addition, a total systems audit would cover all activities shown as well as planning activities (not shown). An audit of the software and hardware to be used should be done prior to input of significant amounts of data. Other audits might be done after the report is prepared to validate the emissions estimate generated.

The checklist is the primary audit tool used by the auditor to help prioritize the audit activities so that the most important phases of the inventory process are evaluated first. Space should be provided on the checklist to record the findings during the audit; however, additional notes may be taken. The checklist is retained and becomes part of the records maintained by the auditor. Because the notes are used to generate the audit report, the auditor should record the findings as legibly and thoroughly as possible.

Four checklists are included as appendices to this volume to provide examples of the approaches an auditor could take when evaluating critical phases of emissions inventories. The questions to consider during the evaluation of the effectiveness of the QC program associated with these critical phases also provide examples of the level of detail in each audit. These questions are based on the procedural and quality requirements included in the inventory work plan and QAP.

After developing the checklist(s) that include(s) questions relative to each critical phase of the inventory process to be audited, the auditor determines the frequency of the audits and when they will occur. The available resources often dictate the frequency of these audits; therefore, the audit schedule should be discussed with the inventory development manager prior to establishing the budget. The auditor should request sufficient funds to provide the oversight needed to achieve the data quality objectives established for the work.

Audits should be conducted throughout the development of the inventory so that deficiencies in the QC program are identified and corrected as soon as possible. Planning the audits in this manner will also foster continuous improvement of the accuracy of the data as the inventory is developed. It is recommended that the audits be conducted at least during the planning stages, during the collection of the data, during the development of the emissions estimates, and after the draft of the inventory is generated. This schedule will provide an assessment of the adequacy of the development activities and QC procedures associated with the most critical phases of the work.

As the schedule develops, the auditor must also determine what type of audit is appropriate to conduct. The auditor may conduct a management systems audit (MSA), technical systems audit (TSA), performance evaluation audit (PEA), audit of data quality objectives (DQA), or
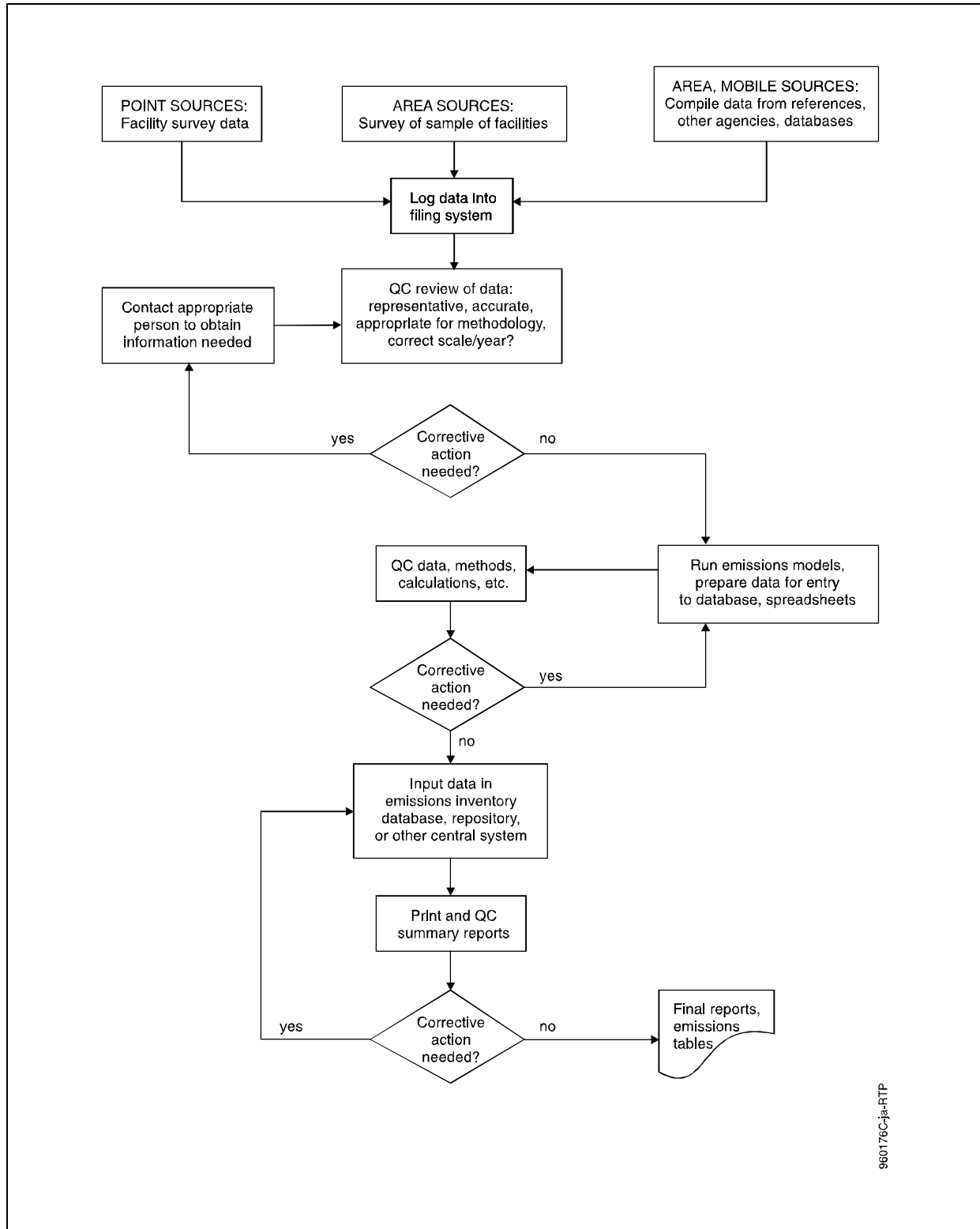
FIGURE 3.8-3. EXAMPLE INFORMATION FLOW CHART

TABLE 3.8-1

OBJECTIVES OF DIFFERENT AUDIT TYPES[a]

Audit Type	Objective
Management Systems	Determine the appropriateness of the management and supervision of inventory development activities and training of inventory developers.
Technical Systems	Determine the technical soundness, effectiveness, and efficiency of the procedures used to gather data and calculate emission results.
Performance Evaluation	Determine whether the equipment used to collect measurement data operates within acceptable limits.
Data/Report	Determine whether the results reported accurately reflect the emission results calculated and recorded in the supportive data.
Data Quality	Determine the accuracy and completeness of the data used to develop the emission results.

[a]See Section 8.2 for more detailed information about these types of audits.

a data/report audit (DRA). The audit type selected depends on the objective of the assessment (see Table 3.8-1).

8.1.4 EFFECTIVE AUDIT PROCEDURES

In order to efficiently use the auditor's time and the time of the inventory development personnel, the auditor should communicate his/her intentions to conduct the audit and hold meetings prior to and after the audit to discuss the audit activities and findings. During each of these steps, notes should be taken to record the information gathered so it can be used to generate the audit report.

The following guidance on effective audit procedures is applicable to all types of audits. However, the relative importance of each step discussed below may vary depending on the type of audit.

Notice of Intent

Approximately one week prior to conducting a systems audit, the auditor should forward a notice of intent to conduct the audit to the inventory development manager. The notice should at least include the following:

- Objective(s) of the audit;

- Proposed date of the audit;

- System(s) or data to be audited;

- Proposed schedule of audit activities; and

- Names of the persons to be interviewed.

This notice helps to ensure that the personnel involved in the critical phases of the inventory process will be available. The schedule of activities will allow the inventory development personnel to plan their activities so that the audit will not interfere with the progression of inventory development activities any more than is absolutely necessary. Identifying the data that will be reviewed also helps save time by allowing the inventory personnel to gather the data and have it available at the time of the audit.

Opening Meeting

At the start of the audit, the auditor holds an opening meeting to discuss the audit plans. During the meeting, the inventory development personnel are introduced to the auditor by the inventory development manager. One week prior to the audit, the inventory development manager may also be asked to provide a brief summary of the inventory development activities so that the auditor knows the status of the development of the inventory prior to conducting the audit. The status of the work may be updated during the opening meeting. The auditor briefly summarizes the intent of the audit and audit schedule. If needed, changes in the audit schedule may occur to ensure that the auditor is able to interview as many of the key personnel as possible. The auditor also informs the personnel attending the meeting of the proposed date/time of the wrap-up meeting, which is held after the audit.

Conduct of the Audit

After the opening meeting, the audit begins. The most effective approach is to follow the natural progression of inventory development: data collection, data evaluation, emission calculation/estimation, and emission results generation. This sequence of events should take the auditor through the critical steps of the inventory process that were identified when

reviewing the planning documents and approved procedures. At each step, the auditor discusses the work with the personnel actually conducting it.

During the interviews or discussions with the inventory development personnel, the auditor asks questions about the systems and data evaluated and compares the answers to the information included in the procedures reviewed during the planning stage of the audit. If approved procedures are not followed, the auditor identifies these occurrences as quality concerns or findings. If responses to procedural questions suggest that personnel training is insufficient, training records may be evaluated to determine if personnel training is a quality concern that may impact data quality.

Likewise, the auditor must consider the operability and ease of use of all instruments used to conduct any of the inventory development activities. This is usually not a concern for inventories developed by an agency using primarily facility data and the emission factor approaches. However, a facility's inventory could involve the use of measured emissions. For example, if the audit includes an evaluation of continuous emissions monitoring of stack emissions, the operation, calibration, and maintenance of the equipment should be evaluated. Equipment maintenance logs should be reviewed to determine if there are recurring problems that could adversely affect the results. After reviewing these records, interviewing the operators, and determining that the operability of the measuring equipment or computers used to calculate emissions is questionable, it should be noted as a finding.

The auditor should plan to spend as much time as possible tracking the receipt, maintenance, and retention of the data gathered and used to estimate/calculate emissions. Some of the major quality concerns found when evaluating emissions data are the lack of sufficient information to verify the accuracy of the emissions results, poor documentation of the supporting data, and the absence of good data management practices. Key questions to ask during the audit to determine the appropriateness of these practices are included in Figure 3.8-4.

As the audit is conducted, the auditor documents the findings on the checklist or in a bound notebook. The notes should be legible and written in sufficient detail to facilitate their use during the development of the audit report, indicate the date the notes were recorded, and include a signature line. The auditor looks for opportunities to praise systems that are working well and personnel who appear to be taking extra steps to control the quality and accuracy of the data since positive feed-back as well as RCAs should be included in the audit report.

Wrap-up Meeting

Wrap-up Meetings are held after the audit to discuss the findings and any other information that may be pertinent for the auditor to know prior to writing the audit report. This

Concerns	Yes	No	Comments
Are the data from the appropriate year?			
Are all of the emission sources identified?			
Is all of the information needed to calculate the emissions results available?			
Are data documented in a manner that will not lead to misinterpretation of the information (e.g., crossing out and obscuring data when making corrections?)			
Are data retained in an easily retrieved manner and controlled so that its location is always known?			
Is black ink used to record data to help reduce the possibility of data loss when there is a need for reproductions?			
Are the procedures used to electronically calculate values clearly explained and are the results reproducible?			
Are the calculated values verified by someone other than the generator?			
Are unit conversions accurate?			
Are the emissions results in the specified units?			
Is the technical approach as indicated in the work plan?			
Auditor:			
Date:			

FIGURE 3.8-4. EXAMPLE DATA AUDIT CHECKLIST

preliminary discussion of the audit findings allows immediate communication of findings that are considered adverse to data quality so that actions can be taken immediately to eliminate them.

The wrap-up meeting is often attended by more personnel than are usually present at the opening meeting. Those personnel interviewed or involved in inventory development activities during the audit may attend this meeting to get immediate feed-back on the audit findings. Senior management may also attend this meeting to get first hand information about the requests for corrective actions and effectiveness of the QC program implemented by the inventory development team.

The auditor should request sufficient time before the meeting to review the notes taken and summarize the audit findings. The goal of the auditor during this meeting is to ensure that the inventory personnel agree that the findings are legitimate concerns that require resolution or corrective actions. The audit findings should be clearly stated along with the impact they may have on the development of a complete and accurate emissions inventory. If additional information can be provided to clarify the auditor's perspective on an issue, it is provided at this time or arrangements are made to provide it soon after the meeting.

8.1.5 AUDIT REPORT

The audit report should be clearly written and distributed to the supervisor/manager of the inventory development activities and the key personnel involved in the audit as soon as possible, but no later than two weeks after the audit. Examples should be given of data, procedures, or systems that are found to be deficient, incomplete, or inaccurate. Examples should also be given of systems that work well and personnel that are doing an exceptional job.

The following information is included in the audit report:

- Identification of the auditor;

- Date of the audit;

- Facility or location of the audit;

- Objective of the audit;

- Descriptions of the system(s), data, procedures audited;

- Names of the persons interviewed;

- Findings (positive feed-back and RCAs); and

- Discussion of follow-up activities that relate to previous audits.

An example audit report is included as Appendix A.

The auditor's goal when reporting an issue found during an audit is to clearly state the concern, the potential impact on the emissions inventory results, and propose a solution or RCA to eliminate the concern. The RCAs should be accompanied by a description of the situation that led to them along with a possible solution to eliminate the quality concern.

For example, if the data for one source was missing, the auditor would indicate that the absence of this information would lead to an incomplete inventory or failure to meet the data quality objective for completeness for a given source. The recommendation could be to use engineering judgment or previous data to estimate the omitted data and flag the results as estimations. The inventory report should include an explanation for reporting estimations rather than results that are based on actual test data.

On the other hand, if an instrument was found to not be appropriately calibrated or tested, or an emissions estimation software system has not been adequately QA'd, the auditor could state that there is a potential for the emissions results developed from this data to be inaccurate. The recommendation could be to qualify or flag the results based on these data to show that they are estimated values because the instrument was not properly tested prior to gathering the supportive data. The auditor could ask the team to evaluate the possible degree of inaccuracy that would be associated with both sets of data given in the examples.

The example included as Figure 3.8-5 could be used to record the RCA and maintain records of the actions taken in response to it. Note that the resolution includes a planned corrective action, identification of the person proposing the action, proposed date of the action, and a description of the action taken.

Follow-up Activities

The auditor must assure that actions are taken in response to the audit findings and that these actions adequately address the quality issues cited in the audit report. Conducting these follow-up activities and determining the recurrence of quality issues are the basis for continuous improvement.

Categorizing the findings helps to identify trends. Trends in the occurrence of quality issues can be used to identify systems that may required additional QA/QC. To promote continuous improvement, the auditor may conduct more system specific audits to determine why the applicable procedures are not producing the desired results. Recommendations can then be made to improve the effectiveness and efficiency of the procedures.

The responses from the inventory development manager concerning the RCAs should include a description of the actions to be taken, identification of the responsible person, and date of implementation. The auditor keeps track of the responses to the audit findings to ensure that they are adequate to eliminate the concerns identified and are implemented within a reasonable time. The time between acknowledgement of the concern and implementation of the action should be based on the severity of the impact on data quality. If there is a possibility that the objective of the inventory will not be met or other data are impacted, actions should be taken immediately to eliminate the concern. If new procedures are to be developed or systems revised, but the concern only has the "potential" to adversely impact

RECOMMENDATION FOR CORRECTIVE ACTION

A. Initial Information

RCA NO:	DATE:	URGENCY LEVEL ☐
ORIGINATOR:	APPROVED BY:	1. Potential for major data loss or information.
ORGANIZATION/INDIVIDUAL RESPONSIBLE FOR ACTION:		2. Potential for failure to achieve data quality objective. 3. Suggested improvement.

B. Problem Identification

SITE/LAB:	SYSTEM:	DATE PROBLEM IDENTIFIED:
DESCRIPTION OF PROBLEM:		

C. Recommended Corrective Action

DESCRIPTION:	IMPLEMENT BY:

D. Problem Resolution

PLANNED CORRECTIVE ACTION:	PROPOSED BY:	DATE PROPOSED:	SCHEDULE IMPLEMENTATION:
IMPLEMENTED CORRECTIVE ACTIONS:			DATE IMPLEMENTED:

E. QA Verification

VERIFIED BY:	DATE:	COMMENTS:

FIGURE 3.8-5. RECOMMENDATION FOR CORRECTIVE ACTION

data quality, the auditor may agree to a longer period between the reporting of the RCA and implementation actions taken in response to it. Regardless of the time interval between the request and implementation of corrective actions, the auditor's job is not done until the quality concern is eliminated. This closure of the issue and frequent audits are the keys to the development of an accurate and complete emissions inventory.

Record Keeping

The auditor should keep all notes taken and information gathered during the audit to provide the supportive data needed to verify the information included in the audit report. A data file should be developed that at least includes the completed audit checklist, notes taken during the audit, technical planning documents that described the objectives of the work and approved procedures, the audit report, and descriptions of actions taken in response to the RCAs.

The records maintained by the auditor are used to monitor the quality of the work during the development of the inventory. Categorizing the findings helps to identify weaknesses in the QC program. This information is also used to plan other audits of systems or data that will help monitor the activities until the number of deficiencies or concerns found during the audit cease to exist or decrease to a reasonable level.

8.2 TYPES OF AUDITS

The preceding description of an audit assumes the conduct of a complete systems audit that evaluates the effectiveness of all systems associated with the development of an emissions inventory. However, other types of audits may be conducted to allow the auditor to concentrate on specific systems or procedures that are critical to the successful outcome of the inventory development activities.

Because most technical studies involve numerous systems that could result in the collection of volumes of data, other types of audits may be needed to provide a more thorough assessment of the adequacy of specific systems or the effectiveness of certain procedures. To accommodate the need for a more thorough assessment of phases of the inventory development process, the auditor may conduct MSAs, TSAs, PEAs, DQAs, and DRAs.

The objective of the audit is used to determine which type of audit is appropriate to conduct. When the auditor needs a qualitative assessment of all or parts of the inventory development process, TSAs may be conducted. During these audits, the auditor can focus on one, several, or all of the procedures and systems. If the auditor is concerned about the adequacy of the devices used to take measurements, a quantitative assessment of the measuring device is needed; therefore, a PEA is conducted. If the auditor is concerned about the manner in which data are recorded and whether it is complete, a DQA may be conducted. Moreover,

the auditor conducts a DRA if there are concerns about the accuracy and completeness of the emissions results and format of the report. Regardless of the type of audit conducted, the auditor plans to conduct the audits throughout the inventory development process to help improve the procedures and data as the emissions results are developed.

8.2.1 MANAGEMENT SYSTEMS AUDITS

Management systems audits are important because the findings can be used to verify the existence and evaluate the adequacy of the internal management systems that are needed to develop a complete and accurate inventory. Generally MSAs are on-site evaluations of personnel management, project management, resources, training, and scheduling. The objective of the MSA is to determine if the work is adequately managed and supervised to meet the objectives of the work. Therefore, the commitment of management to establish and implement adequate QA and QC programs is evaluated. It is important that the evaluation of the QA program is conducted by an external auditor to provide an objective assessment.

Some of the questions that may be included on the checklist used during the conduct of a MSA are as follows:

- Is there an approved QA program that includes adequately trained QA personnel?

- Is the QA program supported and approved by senior management to ensure that actions are taken beyond the reporting level of the inventory development manager to get RCAs implemented?

- Is there a mechanism that allows the QA personnel to keep abreast of the inventory development activities so that audits can be planned at critical phases in the inventory development process?

- Is there evidence of adequate supervision of inventory development activities?

- Does management provide adequate supplies and personnel to get the inventory developed within the agreed upon schedule?

- Have technical work plans and quality plans been developed and distributed to the inventory development staff and QA staff to ensure that the objectives and approved procedures for conducting the work are clearly understood?

- Are routine meetings held throughout the development of the inventory to provide an opportunity to discuss the successes and short-comings that may have arisen during the conduct of the work?

- Is there an effective corrective action mechanism that ensures the elimination of activities that adversely affect the technical and data quality objectives?

During the MSA, the auditor tries to determine if there are adequate management support and appropriate quality programs to ensure that the quality of the work is controlled. Provisions should be made to implement the QA/QC programs as the inventory is developed to ensure continuous improvement and the achievement of the objective of the work.

8.2.2 TECHNICAL SYSTEMS AUDITS

The TSA is a qualitative assessment to determine if the approved procedures applicable to the work are followed. Because these procedures should be described in the planning documents, this audit is conducted to determine if the approved procedures are being followed and how effective they are.

Example procedures and systems that could be evaluated during a TSA and important questions to answer during the audit are included below:

Technical Planning

- Project Organization and Personnel

  -- Is there a sufficient number of adequately trained personnel to conduct the work and meet the deadline for reporting the results?

  -- Does the organizational chart identify the QA Coordinator?

- Are there adequate funds for the resources needed?

- Are the constraints for doing the work outlined in the work plan or QAP?

- Are there procedures and goals for achieving data quality?

- Are technically sound procedures identified and explained in sufficient detail?

- Is there a reasonable inventory development schedule?

Data Collection and Analysis

- Are emission source categories and data elements prioritized?

- Have all emissions sources been identified? How do you know?

- Are data collection procedures adequate?

- Are results calculated in a consistent manner?

- Are instruments used to collect real-time data adequately tested?

- Are the computer software and hardware adequate for their use in managing data or calculating results?

- Are the computer systems validated to be functioning as required prior to each use?

- What procedures are used to verify the accuracy of the calculated results?

Data Handling

- Are data receipt records maintained and tracking numbers assigned to help monitor the completeness of the master data file?

- Is access to the data controlled to help maintain a complete file of all of the supportive data needed to verify the emissions results?

- Are there procedures for handling missing data?

Data Documentation

- Is the information recorded in a manner that will help avoid misinterpretations?

- Are the data documented in a manner that facilitates reconstruction of the development of emission results?

- Are there data correction procedures that help to reconstruct the reason for the correction and ensure the use of the accurate information?

8.2.3 PERFORMANCE EVALUATION AUDITS

Performance evaluation audits are conducted when there is a need to quantitatively assess the accuracy of a measurement system. These audits are infrequently conducted unless there is collection of real-time data to support the emissions results. Sometimes the appropriate corrective actions to take if the operation of the system is questionable are not always apparent; therefore, PEAs are usually conducted in conjunction with TSAs to evaluate the

impact that associated systems may have on the operation and maintenance of the measuring device.

The measurement system evaluated during a PEA could be a continuous emissions monitor (CEM) that is used to determine the composition and concentration of the emissions from a stack located at a chemical plant. During the audit, the auditor determines how close the results from the measuring devices are to the known concentration and composition of the reference material. Sometimes the identity of the audit or reference material is unknown to the operator to help provide an objective assessment of the results.

Regardless of the measurement system, the objective is to determine the:

- The accuracy and precision of the measuring device;

- The acceptability of the QC data collected during routine operation of the measuring device;

- If the device is operating within the established control limit established in the QAP; and

- Changes in the quality of the data between audits or over a specified period of use.

The results are used to evaluate the usefulness of the measurement data in determining emissions results. Measurement data naturally result in the development of a more accurate emissions inventory because actual data are used to perform the calculations.

8.2.4 DATA QUALITY AUDITS

Audits of data quality are conducted to determine the acceptability of the data gathered or developed and used to determine emissions results. During the audit, the auditor assesses the adequacy of the data documentation, collection, review, and management activities. The use of the data to calculate emissions is also evaluated to determine if the technical approach is sound and the conversion of units is accurate.

The auditor should review the results from the quality assessment conducted by the generators of the original data to evaluate the acceptability of data developed externally and forwarded to the inventory developers. If this evaluation is not possible, the results should be qualified by acknowledging that the results were determined from data of unknown quality.

If measurement data are used to calculate emissions, the auditor should review the QA/QC data and determine whether the data are valid for use. The QA/QC data provide important information about sample integrity prior to analysis, sampling technique, sample contamination, and the acceptability of the analytical system. The auditor should review the manner in which the data were flagged to show bias and determine whether the values used to calculate emissions were valid.

Some of the questions that may be asked during this type of audit are listed below.

Data Management

- Is the procedure for logging, filing, retrieving, and storing the data included in a standard operating procedure?

- Are the data logged upon receipt and their use tracked to maintain a complete file of all of the data relevant to the emissions results?

- Are the data retained in one location and access to them controlled (helps to ensure completeness)?

- Are data in the file complete (trace from result back to actual data to see if results are reproducible and supportive data available)?

- Is one person responsible for maintaining the data file?

Data Documentation

- Are data recorded and corrected in a manner that helps to reduce misinterpretation of the information?

- Are data documented in a manner that will render them easy to reproduce, when reproduction is necessary, without risking the chance of losing data because of poor copies?

- Are the name of the data generator and date the data are generated included on each data sheet?

Data Quality Indicators

- Were the data quality goals met?

- How are data gaps eliminated?

Data Generation

- •   Are calculations explained in sufficient detail to reproduce the results?

- •   Are units accurately converted?

- •   Are the results in the required units?

- •   Are procedures for identifying outliers identified and followed?

- •   Are standard operating procedures used to round numbers?

- •   Do results represent the correct year?

Data Processing

- •   Are computer programs documented and validated?

- •   Are programs or spreadsheets tested prior to each use?

- •   Is the accuracy of data transcriptions checked?

Examples of completed work sheets and data audit checklists are included at the end of this section.

8.2.5 DATA/REPORT AUDITS

The data/report audit is a type of systems audit that is conducted to determine the accuracy of the emissions results reported and determine whether there are sufficient data to verify the results. This audit is conducted after the data and report have been checked internally and just before it is forwarded to the requestor. The primary goals of the DRA are to determine whether the report accurately reflects the data and whether the objectives for the work were met by using the approved procedures included in the work plan and QAP. An example DRA checklist is included in the appendix.

Because it is impossible to check every data point reported, the auditor evaluates the complete report and selects key data points that could help assess the accuracy of the remainder of the data. A good understanding of the procedures followed by the data submitters, inventory development team, and reporter helps to conduct an audit that makes efficient use of time and resources.

During the DRA, the auditor attempts to verify the accuracy of all of the concluding statements and raw data included in the report by comparing the data reported to that found in the data file. All of the basic equations used to calculate emissions and the technical approach are confirmed to be as indicated in the approved work plan and QAP. Some of the values are re-calculated to verify the relative accuracy of the emissions data.

In addition, the auditor also determines whether the reporting requirements were actually met.

- Are the results in the required units?

- Is all of the required supportive information included in the report?

- Does the report meet the formatting requirements?

- Is the report dated?

- Are the results from the specified year required to be evaluated?

The questions included in the DQA section are also used to assess the quality of the report and data. The peer review checklist shown in Figure 3.3-1 of Section 3 of this chapter could be used for a DRA.

The DRAs are the last audit to be conducted during the development of the emissions inventory. The information provided by the auditor is used to assess how effectively the QA and QC programs were implemented. The RCAs that require correcting reported values or information are addressed immediately and the auditor remains involved in the corrective action process to ensure that the emissions data are accurately reported. As with all of the audits, information from the audit is used to plan the audit program for the next emissions inventory and help improve the procedures used to control the quality of the inventory data.

8.3 PREFERRED AND ALTERNATIVE METHODS

There are several approaches or methods to follow when auditing emissions inventory development activities. The advantages and disadvantages of these approaches or methods, and the objectives for completing the inventory should be the determining factors when deciding which approach is most appropriate.

For evaluations of inventories developed by state agencies and industry, alternative methods are needed because limited resources or other constraints are inherent to many agencies and facilities developing the inventories. However, before selecting an alternative audit method, one must accept the limited degree of quality that the method will provide. Therefore,

alternative methods for conducting audits should only be implemented when limited resources and other constraints do not permit the implementation of the preferred method or approach.

The preferred and alternative audit methods are included in Table 3.8-2.

8.3.1 INDEPENDENT/EXTERNAL AUDIT

An independent or external audit is conducted by an experienced auditor who is not involved in the emissions inventory development process. The independence of the auditor is signified by the reporting lines to management. In order for the auditor to be independent of the inventory development team and thus be able to provide an objective assessment of the systems and data evaluated, he/she must not report directly to the manager of the inventory development team for performance evaluations. However, it is not necessary that the audit be conducted by another agency or contractor; if the auditor was not involved in the development of the inventory, the audit may still be independent.

During the conduct of independent audits, the auditor must be able to objectively assess the procedures, systems, and data without fear of being reprimanded if the inventory development manager is not in agreement with the findings or RCAs. For this reason, in an organization where quality programs are well-established, the auditor reports to a QA Director or senior management.

Independent experienced auditors will develop an audit program that is of a higher quality than those conducted by inventory development personnel because of their knowledge of effective quality procedures. Successful auditors will also foster good working relationships with the inventory development team. This team building approach is usually encouraged by the auditor to help learn more about the procedures and concerns that the team members may have about data quality. Because of the experience and independence of the auditor, ineffective procedures are more readily identified and more effective solutions are recommended when corrective actions are required. In addition, the independent auditor is better equipped to provide continuous improvement throughout the development of the inventory.

One short-coming to this preferred approach to conducting audits is the need for independence. There could be additional costs if there is a need to expand the inventory team to include an auditor or audit team. However, experienced auditors could help eliminate the costs associated with repeating work because of unacceptable data quality or the incorporation of ineffective QC measures.

Independent auditors could be personnel from other groups or agencies within an organization; therefore, selecting personnel from other groups is highly recommended as a

TABLE 3.8-2

PREFERRED AND ALTERNATIVE METHODS: AUDITS

Method	Identification	Description
Preferred	Independent/External Audit	Audit(s) conducted by an auditor or audit team of experienced quality professionals and technical personnel who do not report to the inventory development team manager or assist in the development of the inventory.
Alternative 1	Internal Audit	Audits conducted by auditors who are also involved in the inventory development process.
Alternative 2	Internal Data Checking	QC checking only by the inventory development team members.

means of providing an objective assessment of the quality of the inventory data and effectiveness of the inventory development procedures. Hiring a contractor with inventory QA experience is another option. Regardless of the source of the auditors, technical as well as QA auditing experience are the keys to implementing a successful independent audit.

8.3.2 INTERNAL AUDIT

Internal audits are conducted by personnel who are engaged in the development of the emissions inventory. Some degree of independence is attained by ensuring that personnel do not audit their own work. For example, a point source inventory developer might audit the area source inventory process. However, because the auditor reports directly to the supervisor or manager, he/she may not be able to provide as objective an assessment of the work as an external auditor would. The reporting lines of authority may also prevent the auditor from resolving issues that may not be favorable to the inventory development manager.

Because the internal auditor is also involved in developing the inventory, he/she may not be able to provide an unbiased assessment of the effectiveness of the procedures or systems evaluated. For example, it is difficult for a writer to edit his work because he often overlooks mistakes that are readily seen by someone who has never seen the document or worked on it. The effectiveness of procedures may also be overlooked because the auditor is

so accustomed to seeing the work conducted in this manner that he/she never considers revising them. Therefore, an internal audit could lead to a higher incident of error because some mistakes or quality issues may be overlooked.

One advantage of the internal audit is that the cost is probably at least partially included in the budget because the auditor is performing technical duties as well as QA duties. Another advantage could be that the auditor is closer to the work so he/she may understand the technical approach and systems better than an auditor who has not been involved in the development of the inventory. The proximity to the work and working relationship with the personnel can also be an advantage that would help to plan and implement the quality program in less time than it may take an auditor who is only involved in the QA aspects of the inventory. However, the decrease in cost associated with these advantages may not be off-set by the probability of a higher degree of errors.

8.3.3 INTERNAL DATA CHECKING

Internal data checking is the most frequent procedure followed to help ensure the accuracy of the inventories; in this procedure, the only "audit" is a review of calculations and procedures by the personnel who originally did the work (or by their colleagues). This method has the highest probable error rate of the three. The error rate is higher because there is no formal quality program that requires assessments of the effectiveness of all of the systems and procedures used to develop the inventory. Examples of the systems that are critical to data accuracy and completeness are management of inventory development activities, personnel training, data documentation, data collection, data retention, and formal corrective action mechanisms. All of these systems or procedures have a tremendous impact on the quality of an inventory.

Internal data checking primarily involves checking the accuracy of calculated results and data transcriptions using the methods described in previous sections of this chapter. It could also include the use of a peer reviewer to evaluate the soundness of the technical approach. This form of QC often does not lead to continuous improvement unless management establishes a mechanism that provides constant feedback of quality issues and corrective actions to the inventory development team.

Continuous improvement also requires the implementation of measures that ensure frequent evaluations of the effectiveness of the inventory development procedures. The results from these evaluations must be documented and reviewed constantly to determine when revisions of the inventory development procedures are required to avoid data loss and inaccurate emissions results. Therefore, the major disadvantages of only incorporating internal data checking as a means of QC are:

- • The absence of a formal quality review program with follow-up activities to help foster continuous improvement; and

- • The absence of a formal means of reviewing the effectiveness of technical procedures and evaluating the negative impact that these procedures may have on the accuracy and completeness of the inventory.

If internal data checking and the development of the technical approach to the work are well planned, if there is supervision of the work, and if the inventory development team is very experienced, the quality of the inventories developed by incorporating this method of QC could be increased. The planning would have to include supervision of work practices and review of the data as the inventory is developed. Communication between managers, supervisors, and team members is critical and QC procedures would have to be implemented to determine when there are activities that adversely impact data quality. Status meetings would also have to be held to keep abreast of the quality issues and actions taken to implement corrective actions.

Incorporating these QC measures and using an experienced inventory development team would make the internal data checking method an acceptable approach to controlling the accuracy and completeness of emissions inventories.

9

EMISSIONS ESTIMATION VALIDATION

QUICK REVIEW

Definition:	Comparison of the estimated (model) emissions to real-world measurements (or surrogates).
Objective:	Prove the correctness of the model, assumptions, and data used to estimate emissions.
Optimal usage:	(1) After model development is complete, but before it is used on a wide scale, and (2) after inventory is completed, but before it is used as basis for decision making.
Minimum expertise required:	High. May require expertise in areas outside of inventory development (such as modelling, sampling, ambient data analysis).
Advantages:	(1) Results in an independent test of an emissions model or inventory, (2) may give insights into areas needing more research, and (3) some methods can be used to identify missing or inadequately represented sources.
Limitations:	(1) Can be labor (and resource) intensive, (2) most methods depend on availability of additional data or models of high quality, and (3) some methods are relatively new, and have their own built-in uncertainties.

9.1 OVERVIEW OF METHOD

The validation of emission estimates is the ultimate tool for assuring the quality and, more importantly, determining the accuracy of emission estimates. Validation can be used to "prove" (ideally using statistical methods) the accuracy of an emissions model for a specific category. Also, some methods can be used to validate entire inventories.

All validation methods rely on independent measurements, but not necessarily direct measurements of emissions. Surrogate variables known to be correlated with the emission activity may be measured, or ambient concentrations may be measured. In the latter case, additional modelling is generally used in the analysis; these models have some uncertainty associated with them, however.

Furthermore, field measurement and receptor modeling methods offer completely independent checks on emission inventories since the methods rely on monitoring data alone to estimate either the direct or relative contribution of emissions from individual sources (or source groups). The inverse modeling techniques are not totally independent because they use the emission estimate as the starting point for the air quality modeling. However, output of the model is the best-fit adjustment required to the emissions inventory to allow the modeled concentration data to match observed ambient concentrations. Thus, each method provides the emissions inventory analyst the tools to verify the relative or absolute emissions estimated through the emission inventory process and identify potential problem areas, weaknesses, and strengths in current inventory methodology.

Validation methods should only be used to evaluate and/or calibrate a thoroughly QA/QC'd model. They are not substitutes for the standard QA and QC procedures described in previous sections of this chapter. Moreover, because of the potentially high cost of validation procedures, attempting to validate an inventory that has not been thoroughly QA'd can result in false results and a waste of resources.

Because the procedures described here are relatively expensive, require expert skill, and, in some cases, are fairly new and not entirely accepted by the inventory community, the EIIP considers these an optional component of an emissions inventory QA program. At the same time, the EIIP encourages the continual development and use of validation methods. Studies such as the ones described below are ultimately the best way to determine the accuracy (and in particular, the bias, see Chapter 4) of emission inventories.

9.2 DIRECT AND INDIRECT MEASUREMENTS

Direct and indirect measurement methods involve field measurement of actual emissions or surrogate parameters highly correlated with the emitted pollutant. These measurements can be used for two purposes. First, the data can be used to verify and evaluate emission

models. Second, the field data can be processed to produce direct estimates of emissions and emissions uncertainty for the sources measured (See Chapter 4). Because of their ability to provide unique sources of information on emissions, field studies have the potential to significantly enhance the understanding of the processes producing emissions and the uncertainty in these emissions.

Prior to using field data to calculate emissions, develop emission factors, or model the data to enhance an understanding of the emission process, one must evaluate the accuracy of the raw data used to generate the field data report. This evaluation should include reconstruction of the work and verification that the field/laboratory work was technically sound and the data points are accurate. The QA/QC information provided with the reported results may also be reviewed to assure that the results are of sufficient quality for their intended uses.

Evaluation of original field data often allows the reviewer to evaluate the bias, if any, associated with each data point. Bias may be related to field sampling techniques, sample contamination, or an unstable measurement system. To assess the validity of the data points, QC sample results or results from the analysis of blanks, matrix spikes, duplicate samples, replicate sample, or instrument calibration check samples can be evaluated. The intended use of the data should be used to determine the appropriate level of review needed. See the levels of inventories based on their intended use in Table 2.1-2 of Chapter 2 of this document.

A well-known field study is the "tunnel study" of Pierson et al. (1990) in which motor vehicle emissions were estimated from air pollutant concentrations measured within the Van Nuys highway tunnel in Los Angeles. The results of this study seemed to indicate that the available emission factors model in use at the time significantly underestimate VOC emissions from motor vehicles while NO_x emissions seem to be estimated satisfactorily. However, the interpretation of these data have been questioned by EPA and others and the results are subject to debate.

Remote sensing has significant potential for use in estimating both point source and area source emissions and emissions uncertainty in industrial settings. For example, Spellicy et al. (1992) used Fourier transform infrared (FTIR) spectrophotometry to estimate speciated VOC concentrations due to emissions from area sources within a petrochemical complex. When these data are correlated with process information and meteorological data, estimates of emissions and emissions uncertainty can be developed.

Indirect measures also provide significant information that can address emission uncertainty issues. For example, Claiborn et al. (1995) released a surrogate tracer species (SF_6) to measure the relative dispersion of the tracer and PM_{10} from paved and unpaved roads. The ratio of the measured PM_{10} and tracer concentrations and the tracer release rate was then used to estimate emission factors for PM_{10} emissions from the roadways. Estimates of

uncertainty can then be determined directly from the field measurements. These tracer methods make the fundamental assumption that the tracer is emitted and disperses in the same manner as the pollutant of interest. This assumption may not hold in some situations so care must be taken when performing tracer studies and when analyzing the study results to ensure that this key assumption is met.

Fujita et al. (1992) estimated ratios of various pollutants developed from emission inventories and ambient monitoring data from the South Coast Air Quality Study (SCAQS). Table 3.9-1 presents results from Fujita et al. in which they compared the ratio of ambient and emission inventory estimated ratios of CO/NO_x and $NMOC/NO_x$. Included in Table 3.9-1 are the adjustment factors to the exhaust portion of the emission inventory that would be required to bring the emission inventory ratios to equality with the observed ambient ratios (i.e., remove a potential bias). Based upon this analysis, they suggested that VOC from motor vehicles, relative to NO_x, appears to be underestimated in motor vehicle emission inventories, the same conclusion reached by Pierson et al. discussed above.

Janssen and Koerber (1995) have also compared computed to observed VOC to NO_x ratios as part of the Lake Michigan Ozone Study (LMOS) in an effort to understand uncertainties in the LMOS emission inventory. Their initial analysis of VOC/NO_x ratios indicated differences of more than a factor of two with the estimated ratio higher than the observed ratio. However, after a prioritized review and reassessment of the sources of VOC emissions contributing most significantly to the estimated ratio, the difference between the observed and estimated ratio was reduced to under 30 percent. This study is a good example of the role that observed monitoring data can play in prioritizing enhancements to emission inventories.

Peer et al. (1992) used field sampling data to develop a regression model and to validate and calibrate a physical model of emissions of methane from landfills. In this study, data from 21 landfills with gas recovery systems were collected and used to develop a regression model of methane emissions. Information included in the model were methane recovery rate, landfill size, refuse mass, site age, and climatic measures (average precipitation, temperature, and dewpoint temperature).

The data for each landfill were also used to validate the EPA's Landfill Air Emissions Estimation Model. This model is used to estimate methane (CH_4), carbon dioxide (CO_2), and VOC emissions for individual landfills; it is sensitive to the input values for k (decay rate) and L_0 (methane potential of the waste). Table 3.9-2 shows a comparison of the performance of the deterministic model and the regression model. The numerical values shown are the ratios of actual methane flows (at each of the 21 landfills identified by "site number") to predicted methane emissions for the models. The closer the ratio is to 1, the better the predicted value.

TABLE 3.9-1

COMPARISON OF AMBIENT AND INVENTORY RATIOS OF CO/NO$_X$ AND NMOG/NO$_X$ FOR LOS ANGELES FOR 1987

Pollutant Ratio	Season	Time (PST)	Amb/EI Ratio[a]	Required MV Adj Factor[b]
CO/NO$_X$	Summer	06 - 08	1.4	1.5
		20 - 08	1.6	1.9
	Fall	06 - 08	1.1	1.2
		20 - 08	1.4	1.7
NMOG/NO$_X$	Summer	06 - 08	2.5	4.4
		20 - 08	3.0	5.5
	Fall	06 - 08	1.7	2.8
		20 - 08	2.3	4.0

Source: Fujita et al., 1992.

[a] Ratio of the pollutant ratio estimated from ambient monitoring data to that estimated from the motor vehicle emissions inventory.

[b] Adjustment factor required to bring the hot motor vehicle emissions inventory ratio to equality with the ambient ratio.

The Landfill Air Emissions Estimation Model was run using three different sets of input values for k and L$_0$; Run 3 used the recommended defaults. Based on this study, these defaults were shown to overpredict emissions (mean ratio is 1.97). Subsequent versions of the model recommended new default values similar to the input values used for Run 2.

Field studies provide the information needed for direct estimates of both emissions and the uncertainty associated with those estimates. However, there are two significant limitations of field studies that must be addressed in any field program. First, the emissions data are only valid for the conditions and sources that were present during the field measurements. Because it is not possible to make measurements under all conditions for all sources, there are inherent biases that will be present in all emission models developed based on the field data if these models are applied outside the development bounds. For example, if the traffic in the tunnel during the Van Nuys tunnel study were atypical of traffic in the Los Angeles area and that represented internally in the emission factor model, the results of the analysis of the data from the study would have limited applicability.

TABLE 3.9-2

VALIDATION OF LANDFILL METHANE EMISSIONS MODELS[a]

Site Number	Landfill Air Emissions Estimation Model			Regression Model
	Run 1 Pred./Actual	Run 2 Pred./Actual	Run 3 Pred./Actual	Pred./Actual
1	0.16	0.40	0.73	0.52
2	0.48	1.21	2.23	1.55
3	0.28	0.71	1.31	0.83
4	0.22	0.55	1.01	0.62
5	0.58	1.44	2.66	1.95
6	0.24	0.60	1.10	0.73
7	0.46	1.16	2.14	1.50
8	0.37	0.93	1.71	1.15
9	0.36	0.90	1.67	1.15
10	0.25	0.64	1.17	0.83
11	0.23	0.57	1.05	0.85
12	0.54	1.34	2.47	1.72
13	0.16	0.39	0.72	0.57
16	0.33	0.82	1.52	1.02
17	0.49	1.23	2.26	1.73
20	0.41	1.02	1.88	1.24
21	0.15	0.36	0.67	0.47
22	0.19	0.47	0.87	0.57
23	1.74	4.35	8.00	6.32
24	0.54	1.34	2.46	1.60
25	0.82	2.06	3.79	2.34
Mean	0.43	1.07	1.97	1.39
Standard Deviation	0.34	0.85	1.56	1.24

[a]From Peer et al., 1992.

A second limitation is that field studies must limit their effort to generally well-defined source classes or source types. It is not possible to design a comprehensive field program to measure all, or even most, of the emission sources in an urban area. Consequently, there will be inherent limitations in the applicability of any emission model or uncertainty estimates developed using the data.

9.3 RECEPTOR MODELING

Receptor modeling, also called source apportionment, is a "top-down" method of estimating the relative contribution of individual source categories to an emission inventory. The Chemical Mass Balance Model (CMB) (Watson et al., 1984) is a widely used model for performing receptor modeling. It is called top-down because it uses information about the entire inventory and modeling domain to estimate the relative contribution of emissions from each source category rather than building up contribution estimates on a source-by-source basis.

In receptor modeling, least squares estimation is used to obtain the best fit of emissions from each source modeled that reproduces the chemical composition of observed monitoring data at a given monitoring site. The two key input requirements for receptor modeling are the chemical composition of ambient monitoring data and the chemical composition ("fingerprints") of emissions from each source with the corresponding same level of detail as the monitoring data.

The model is able to resolve contributions from sources that have unique chemical compositions. Unless a given source (facility) has a unique emissions chemical composition, it is not possible with receptor modeling to resolve the impact of an individual source. In addition, only relative impacts are produced by the model indicating the relative contribution from each source class. Typical source classes modeled include motor vehicle exhaust, fuel combustion, electric utilities, construction activities, marine aerosol, and fugitive dust of geological origin.

Receptor modeling in the past has been used primarily for examining sources of relatively stable pollutants such as particulate matter. For example, Chow et al. (1992) used the CMB to examine PM_{10} source apportionment in the San Joaquin Valley in California. They concluded that fugitive dust of geological origin (e.g., fugitive dust from agricultural tilling, roadways, and construction activity) exceeded 50 percent of the observed PM_{10} at Bakersfield in the summer and fall. Onroad motor vehicles contributed only approximately 10% of the observed PM_{10} while 4 percent of the PM_{10} mass was unexplained.

Much recent work has been performed to apply receptor modeling to reactive pollutants. For example, Scheff et al. (1995) applied the CMB to evaluation of emissions of non-methane

organic compounds for the Southeast Michigan Ozone Study (SEMOS). Sheff selected chemical species with relatively low reactivity for use in the modeling, and selected his modeling scenarios to reflect relatively small travel times. Using this methodology, Sheff et al. were able to overcome the issue of reactivity and loss of emitted mass times and thus limited the potential influence of atmospheric photochemistry on the modeling results. They concluded that the relative proportion of the observed NMOC concentrations was consistent with current estimates of emissions for architectural coating and coke oven sources. However, there were significant differences between the CMB results and the current inventory on the relative proportion of emissions from refineries and graphic arts.

A limitation of the methodology is the resolution available from the CMB model is limited by the quality of the available source emission composition profiles. Because of the large variability between sources and potentially from test to test for a given source, these profiles are highly variable. Consequently, significant preparatory work must be performed to ensure that the most representative source profiles are used as input to the CMB model. In addition, the monitoring data used in CMB modeling must be representative of ambient concentrations in the area in which the emissions are occurring. These monitoring data cannot be primarily influenced by local sources for which source profiles are not available. Nor can chemical reactions or losses such as deposition or decay deplete the emitted substances prior to their measurement as ambient concentrations.

9.4 INVERSE AIR QUALITY MODELING

The inverse air quality modeling method relies on the use of a validated air quality dispersion model to back calculate what the emissions should be to produce the observed air pollutant concentrations. These general inverse methods are based upon an iterative application of a Kalman filter (Hartley and Prinn, 1993). They use a recursive, least squares approach to minimize the difference between the observed concentrations field and the modeled concentration field produced using adjusted emissions. These methods are very powerful and can yield direct estimates of temporal and spatial emissions and their uncertainty, both overall and stratified by source type or location.
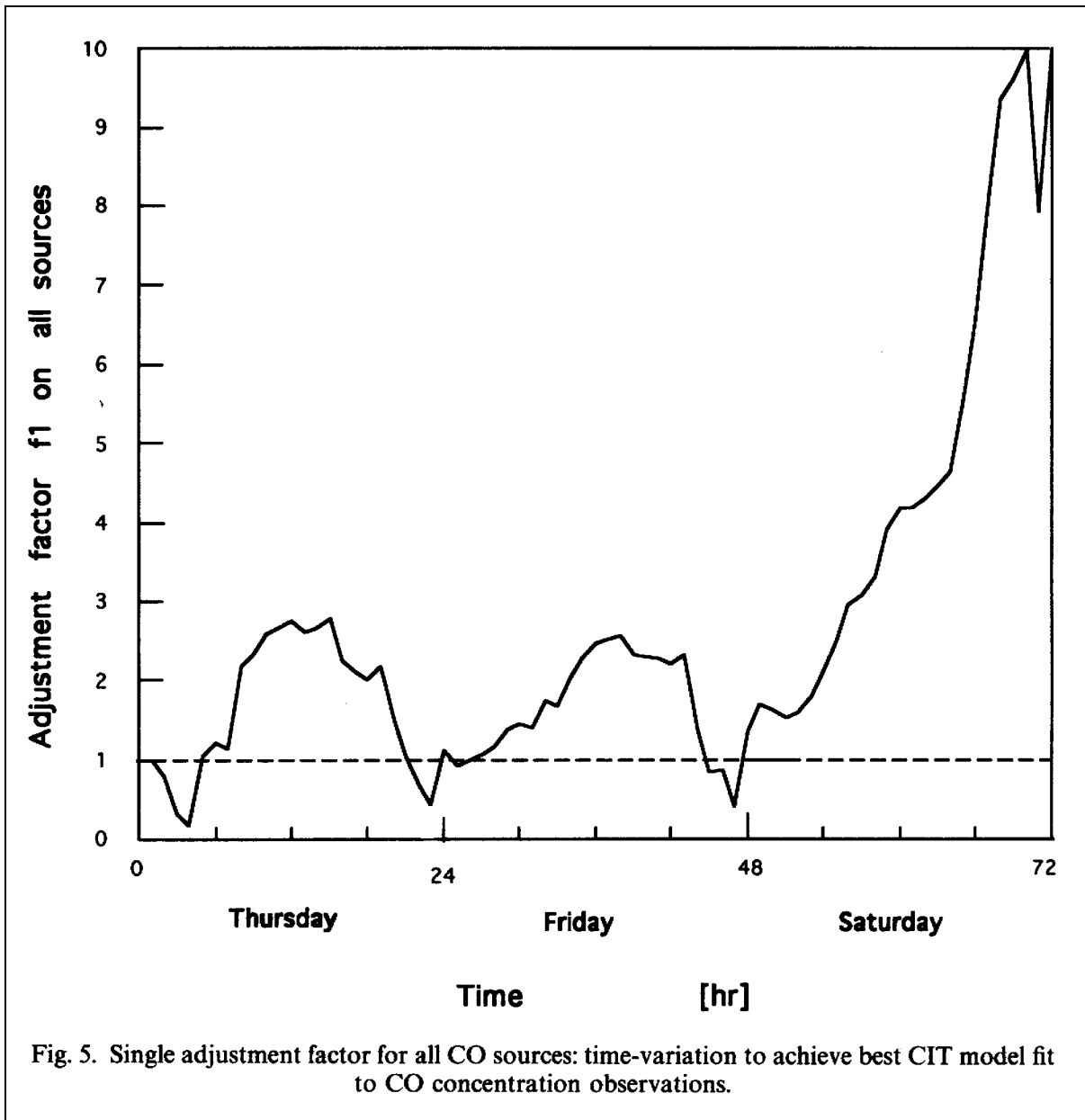
Chang et al. (1993; 1995) used the Kalman filter approach to examine the ability of this methodology to yield estimates of emission uncertainty. Work in progress is continuing the testing of this methodology and applying it to estimate uncertainty in isoprene emissions in the Atlanta area (Chang et al., 1995).

Mulholland and Seinfeld (1995) used the Kalman filter inverse modeling approach to examine potential errors in the CO inventory for the Los Angeles area. In this study, estimates of both temporal and spatial errors in the CO emissions inventory for Los Angeles were developed. Figure 3.9-1 presents the estimated overall temporal adjustment factor for air basin-wide CO emissions that resulted from the best fit between the modeled and

observed CO concentrations. The weekday adjustment varies from approximately a factor of 3 during the day to considerably less than one at night. The weekend adjustment factor approaches a factor of ten. In addition to these temporal biases, they also identified potential spatial biases in the Los Angeles CO emissions inventory, including a postulated significant underestimate of recreational traffic along the coast on the weekend day modeled (Saturday).

There are inherent limitations in the use of air quality models for estimating emissions uncertainty. Air quality simulation models are imperfect representations of the real world in that many simplifying assumptions must be made during model development. These models, in their attempt to simulate very complex atmospheric behavior, introduce their own uncertainty to the emission estimates. These uncertainties can be due to inherent assumptions in the model, the numerical algorithms used to implement the assumptions, inadvertent biases introduced in the model formulation, and imprecise or erroneous input data. As a result, there are limitations to the accuracy of air quality models in use today.

Any use of the inverse air quality modeling methodology to estimate emissions uncertainty must account for the uncertainty introduced by the air quality model itself. For example, the EPA performance goal for the Urban Airshed Model is for the gross error of all observed-predicted pairs to be less than 30 to 35 percent and normalized bias to be within ±15 percent (U.S. EPA, 1991b). However, when the model is used to examine differences between modeling scenarios or incremental differences in model estimates due to small perturbations in model input (such as occurs in these general inverse methods), the model errors and biases can tend to cancel or drop out. Consequently, the uncertainty introduced into the estimates of emission uncertainty can be made small compared to the other sources of uncertainty.

Fig. 5. Single adjustment factor for all CO sources: time-variation to achieve best CIT model fit to CO concentration observations.

FIGURE 3.9-1. SINGLE ADJUSTMENT FACTOR FOR ALL CO SOURCES

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