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PROCEDURES FOR VERIFICATION OF EMISSIONS INVENTORIES

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Research Triangle Park, NC 27711

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In many cases, pertinent examples of a specific approach or the application of such have been provided in the text, to facilitate the transfer of verification ideas to other programs. The author was responsible for selection of those examples and recognizes that there are numerous other examples that have been overlooked or omitted entirely. Apologies are offered for these oversights, and the fact that some examples are not referenced in this report does not imply that those approaches or ideas are not of value. The fact that other approaches are available is merely an indication that interest in emission verification techniques is increasing and will continue to grow in future programs.

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PROCEDURES FOR VERIFICATION OF EMISSIONS INVENTORIES

BACKGROUND AND OBJECTIVES

INTRODUCTION

The Task Force on Emissions Inventories was commissioned by the United Nations Economic Commission for Europe (UN/ECE) in the spring of 1992. The Task Force, comprising environmental professionals from 24 countries and six international organizations, agreed to a three-year work plan to develop information requirements to prepare emissions inventories for European countries and to establish procedures to ensure compatibility and transparency among the inventories developed for these nations. The Task Force established eight Expert Panels to address the principal needs in specific areas of interest to the Task Force. These Expert Panels are listed below:

- The Strategic Overview Expert Panel
- The VOC Expert Panel
- The Ammonia Expert Panel
- The Expert Panel on Heavy Metals and Persistent Organic Compounds
- The Power Plant and Industry Expert Panel
- The Mobile Source Expert Panel
- The Marine Expert Panel
- The Verification Expert Panel

Each Expert Panel was charged with preparation of a contribution to *The Atmospheric Emission Inventory Guidebook* to identify the issues and to summarize approaches to be followed in emissions inventory programs in Europe. This report is a compilation of the information and techniques discussed by The Verification Expert Panel. The report discusses some of the principles of emissions inventory preparation and the techniques and procedures that can be applied during the planning and development of emissions inventories to increase the accuracy and reliability of emissions estimates. Methodologies that have been applied in previous emissions inventory projects and additional proposed activities to validate the emissions inventory data are discussed.

Although the information discussed in this report was prepared for application by the nations participating in the UN/ECE Task Force, the issues and approaches discussed are relevant to any emissions inventory development project. The summary of approaches and techniques can be used to document data quality and to establish confidence in emissions estimates in State, national, and global applications.

An emissions inventory is the foundation for essentially all air quality management programs. Emissions inventories are used in two primary applications by air quality managers. The first use of emissions inventories is in assessments that identify the largest air pollution sources in a region. The second use of inventories is in regulatory and policy making applications including as input data for air quality models, and in the development, implementation, and tracking of control strategies. Each of these uses provides information that is needed by decision makers to establish priorities and to make effective air quality management decisions. A number of approaches can be used to compile emissions inventories, and the selection of an appropriate technique is largely dependent on the needs of the specific program, the personnel and funding resources available for the program, and the schedule constraints that are placed on the program. Because emissions inventory data are usually estimates, it is always desirable to provide an assessment of the validity of the estimated emissions magnitudes as a component of emissions inventory development projects. The emissions validation or verification process assists decision makers in choosing appropriate regulatory options.

Public awareness of the health and other environmental problems associated with industrialization have made air quality management problems a high priority in some European countries where these issues have not been a high priority in the past. Many of the important air quality issues are regional in scope and may require emissions inventories that cross country borders. Inventory verification is particularly important for programs involving multiple countries with different levels of resources for inventory development.

The purpose of this document is to provide guidance related to the development of emissions inventory data and suggestions for procedures and techniques that can be used to assess the validity of the emissions data included in the inventories. Since most emissions data are estimates, it is often difficult to derive statistically meaningful quantitative error bounds for inventory data. Frequently, it is possible, however, to provide ranges that bound the likely minimum and maximum for an emissions estimate or to develop a qualitative data quality parameter to indicate the relative confidence that can be associated with various estimates.

This report begins with a background discussion of the approaches for emissions inventory development and the role of emissions inventory data in air quality management activities. Considerations applicable in planning phases of inventory development efforts that can improve the reliability of inventory data are discussed. The remainder of the report discusses specific analyses that can be performed to assist in validating emissions inventories.

HISTORICAL PERSPECTIVE

Over the past two decades, the industrialized countries in North America and Europe have cooperated on air quality management programs. Air quality standards, that set ambient concentration limits for air pollutants, are a cornerstone of these programs. Air quality standards are established to protect public health, and to limit other impacts of air pollutants on agriculture, structures and other economic interests. Coordinated research to identify appropriate emissions control options were developed to reduce the amount of pollutants that are emitted to the atmosphere, as a control strategy to achieve the ambient concentration limits. The following discussion briefly summarizes the history of these programs in the United States as an example of similar programs that have been implemented in many of the other industrialized countries.

Originally, the United States established air quality standards for sulfur dioxide (SO_2), nitrogen dioxide (NO_2), carbon monoxide (CO), total suspended particulate matter (TSP), and photochemical oxidant expressed as ozone (O_3). The U.S. EPA provided guidance for the control of air quality to achieve these ambient standards. Most of the oxidized nitrogen is emitted in the form of nitric oxide (NO). Atmospheric reactions can rapidly convert NO to NO_2, and emissions control programs for NO_2 were based on limiting emissions of total oxides of nitrogen (NO_x). Ozone and the other primary photochemical oxidants are not emitted directly from sources but are formed through a complex reaction sequence involving nonmethane hydrocarbons (NMHC) and NO_x in the presence of solar ultraviolet light. In the United States an ozone control policy, based on the control of emissions of NMHC, was adopted. Many other countries have adopted similar ozone control policies.

Since the original definition of the criteria pollutants, the nomenclature for NMHC has changed to volatile organic compounds (VOCs), the PM standard has been changed to an ambient concentration standard for particulate matter of aerodynamic diameter less than 10 microns (PM-10), and a NAAQS standard for lead (Pb) has also been established.

Throughout the 1970s and 1980s, air quality management in the United States, and other countries, was perceived as a local problem, and local jurisdications were charged with the responsibility for the development and implementation of air quality control programs. National programs were established in most countries, to provide guidance and to support the local agencies. In the United States, EPA conducted research on source-specific control techniques and mobile source control to assist the local agencies in developing their air quality management plans.

Emissions control research focused on the emissions processes of individual source types. This research led to the compilation of recommended source-specific emission factors for each of the important air pollution species. The recommended emission factors developed in the United States, were published in the document entitled *Compilation of Air Pollutant Emission Factors, Volume I, Stationary Point and Area Sources, AP-42.*[1] This document has been revised through the years and is currently undergoing another revision; it will soon be released in its fifth edition. Emission factor compilations similar to the *AP-42* have been used by many countries to develop emissions inventories.

The procedures recommended for emissions inventory development generally involve the application of a representative emission factor that relates the magnitude of air emissions to some other operating parameter associated with the activity. The emission factors are specified in units of pounds of emissions per unit of that specified activity. Some common examples include emission factors that are expressed in terms of the number of tons of coal burned, the number of barrels of oil refined, tons of chemical produced, tons of solvent consumed, square feet of surface coated, vehicle miles travelled, density of biomass, number of employees, the population of a geopolitical unit, and acres of harvested land. In general, the activity data required for emissions inventories for industrial sources are known at the annual level with a great deal of confidence. The activity data for consumer- based source categories, such as the use of personal hygiene products, lawn and garden care products, and household consumer products, however, are generally not as well known and are often estimated. Since a large amount of inventory data is based on estimates, there is commonly a large amount of uncertainty in the final emissions inventories.

CURRENT PERSPECTIVE

Unfortunately, air quality issues rarely involve analyses of annual emissions of a particular pollutant. The effects of poor air quality are more commonly associated with repeated, short term occurrences of high concentrations of pollutants. The most intractable of these issues in industrial countries also involve complex interactions of emitted pollutants with atmospheric systems that result in the generation of secondary pollutants. Examples of problems related to secondary pollutants are ambient ozone that is formed through complex chemical interactions involving VOC, NO_x and solar ultraviolet radiation, and the production of acidic deposition species through interactions of SO_2, NO_x, ammonia, and other alkaline components. Coordinated air pollution research over the past 20 years has led to the development of analysis tools including air quality models and statistical data analysis techniques. These analysis tools require emissions data that are at a finer level of spatial and temporal resolution than the data of the original estimates. Emissions data often need to be formatted in a regular spatial grid pattern that represents the region for which the inventory was developed. The emissions data are also often required at daily or hourly levels of resolution. Finally, since the individual components that make up the VOC and PM-10 often have different effects on secondary pollutant formation, the emissions estimates must be resolved (speciated) to represent their chemical composition. Each of these steps of resolution requires assumptions and estimates of the distribution functions, which are seldom well known, thereby adding uncertainty to the emissions estimates that are ultimately used to evaluate control strategies.

The largest sources of air pollutants were considered for control in the early efforts of air quality management. Overall, control programs for the major sources have resulted in significant reductions of emissions, and the existing air quality in the countries with aggressive control programs is considerably improved relative to the conditions that would be present if no controls had been implemented. The effects of increased population and expanded industrial development, however, continue to produce emissions that cause air quality standards to be exceeded and public health to be threatened. Inventory-based control plans have been successful in reducing the number of urban areas that violate air quality standards, and in terms of the number and severity of violations of air quality standards in many locations. This success has not been universal, however, and additional pollution control is necessary to achieve complete success. As a result, air pollution control programs must be expanded to include small sources and other activities that have not been regulated in the past. These requirements place increased emphasis on the preparation of complete and accurate inventories of the emissions sources in urban areas that are in violation of air quality standards. Activities to promote pollution prevention, recycling, and conservation are key components in programs to identify achievable emissions reductions from the previously unregulated sources and source categories.

The needs related to allocating emissions data to the resolution required by air quality models and the need for improved emissions estimates for a larger number of small sources have increased the demand for reliable emissions estimation techniques and for appropriate verification methodologies. Emissions inventory verification programs will not only provide information useful to air quality decision makers, but will also help to prioritize future activities for inventory improvements.

EMISSIONS ESTIMATION AND THE SCALES OF AIR QUALITY ISSUES

The concept of emission factors and the fact that almost all emissions inventories are based on the application of emission factors has already been presented. There are, however, several approaches for estimating emissions that rely on the use of emission factors. All of the approaches can be categorized as being either top-down or bottom-up. The top-down process involves the estimation of the inherent activity at a highly aggregated level of resolution such as at the country, or provincial level. In the bottom-up approach attempts are made to estimate emissions for individual sources and other specific human activities. These individual estimates are then summed to represent the total emissions. The choice of the specific emissions estimation approach to be used depends on the scope of the project, the data requirements, the resources and schedule constraints, the amount of data available, and the level of detail represented in the available data.

Obviously, it is preferable to produce a detailed bottom-up inventory for application to modeling activities and area-wide control strategy development. The amount of uncertainty associated with the modeling emissions inventories is decreased if source-specific information can be obtained. Similarly, if specific source operating conditions are known, the benefits and costs of emissions control can be evaluated in more detail than is possible if only a national average emission estimate is available. The methods and techniques that can be applied to emissions verification efforts are also dependent on the type of methodology used to develop the inventory.

Emissions from large point sources, mobile sources, dispersed area sources, and biogenic and other natural sources are all important in the atmospheric processes that result in air quality problems. The needs associated with emissions inventory development projects depend on the type of air quality program to which they will be applied. National assessment of the major sources would require only annual estimates of the total contribution of pollutants by major industry types, whereas a study to evaluate the health impacts of a proposed industrial facility would need hourly operating rate data and specific pollutant emissions anticipated from the proposed industrial process. The degree of accuracy and precision, and the type of emissions inventory verification program that is applicable to these problems is in turn related to the inventory needs.

Historically, air quality problems have been addressed through pollutant specific regulatory responses that are implemented and enforced independently. The general approach to addressing these issues was to identify the specific health or environmental effect, evaluate the pollutant emissions that contribute to that effect, and implement economically achievable controls to reduce the emissions of the pollutants. These problems are now known to involve interactions among primary source emissions, atmospheric processes, long-range transport and transformation, wet and dry deposition, and ecological feedback systems. Air quality problems can be thought of as occurring in the four regimes listed below.

- Local, source-specific problems occur over a period of hours to a day, during which primary pollutants emitted from a source have acute and cumulative toxicity effects on the population in the immediate area. The pollutants of interest in this regime are not influenced by chemical reaction.

- Urban area problems involve the collection of emissions sources in an urban area and the interactions of those emissions with one another. These interactions occur under the influence of local meteorological conditions to produce secondary pollutants that have health-related implications to the population in the urban and surrounding areas. The primary examples are violations of the ambient ozone and CO standards. These issues involve photochemistry and other complex atmospheric chemistry processes that take place over a period of one to three days.

- Regional air quality problems are those that occur on the scale of major weather systems and generally involve transport conditions where the effects can occur at distances of up to 1,000 kilometers from the source areas. These types of problems occur over periods of several days to more than a week and may or may not involve atmospheric chemistry. The examples are elevated rural ozone concentrations, air toxics deposition, and acid deposition problems.

- Global air quality problems occur over periods of years. These problems involve the collective emissions of species from all countries. The compounds of interest in global problems are subject to atmospheric removal processes that are slow relative to the global emissions rate. Global climate change and stratospheric ozone depletion are examples of these problems.

Often the individual problems included in each of these regimes are related to one another. In particular, the oxidation chemistry associated with urban ozone formation processes can affect and are influenced by several of these other processes. Obviously, regional rural ozone concentrations are affected by the emissions of VOC, NO_x, and CO that initially occur in and around the urban centers. The same species that oxidize VOCs in the ozone formation process also affect the oxidation of sulfur and nitrogen compounds in the formation of acid deposition species. The photochemical processes that occur on urban scales can also affect the global distribution of radicals and other intermediate species that can influence the concentrations and removal rates of species active in the global problems.

All of the issues concerning emissions inventory preparation and the uses of emissions inventories summarized above influence the decisions that affect the approach that will be followed to validate the emissions inventory. An emissions verification program can range from simple efforts that compare total national emissions per person to those of other similar countries, to detailed emissions range estimations for specific sources. Each is useful to add credibility to the estimates and to prevent inappropriate applications of the resulting data.

CONCEPTUAL ISSUES OF EMISSIONS VERIFICATION

The preceding discussion emphasized the importance of appropriate emissions inventory estimates to the success of air quality management and decision making. Of equal importance are the procedures that will be included in the effort to ensure the accuracy, completeness, and representativeness of the emissions data. These activities are collectively referred to as quality assurance and are implemented through a quality assurance plan. Each air quality analysis effort has specific emissions inventory needs that are related to the scale and objectives of the program. In most applications, it is highly desirable to include in the program design methodologies and procedures to ensure and document the quality of the emissions data. The effort that is appropriate for these quality assurance and data verification components is dependent on many factors. Primarily, considerations of the objectives of the program and the resources available for the program influence the decisions on what type of quality assurance and verification effort are reasonable.

An emission verification program is inherently related to quality assurance procedures and objectives, but the concept of emissions verification extends beyond quality assurance activities. Quality assurance procedures are defined and followed to ensure that the data that serve as the foundation for the emissions estimates are the most representative, complete and meaningful data available for the intended application. An emissions validation or emission inventory verification program is performed to test how well the completed emission inventory supports correct decision making in air management planning. As such, a verification program will provide data that can be applied to demonstrate that the final emissions inventory is useful for its intended application, rather than to provide data to test the accuracy of emissions or operating data for individual sources.

This report presents the elements that should be considered in the development of an emissions inventory and in the quality assurance aspects of inventory development efforts to establish the validity of the emissions data. Whenever possible, examples of some quality assurance activities that have been performed in emissions inventory programs in the United States and Europe have been presented. Some of these examples are derived from the experience obtained during the development of the National Acid Precipitation Assessment Program (NAPAP) emissions inventory and in the preparation of emissions inventories used by the State agencies and EPA in developing air quality control plans for criteria pollutants.[2,3]

This report is intended to represent a comprehensive discussion of verification concepts and approaches that can be applied before, during, and after the development of emissions inventories to improve the usefulness of emissions data. Ideally, some of the verification techniques discussed here should be completed by the inventory developer and presented along with the inventory databases to establish reliability and usefulness. If program resources and time schedules prohibit the completion of these tasks by the developer, users and/or third party reviewers can complete these tasks with equal credibility if the procedures followed in the development of the inventory are adequately documented.

These approaches include some techniques that have been widely applied in past programs and others that are experimental and have only been applied in selected applications. The concept of a coordinated emissions verification program using a mix of routine and experimental techniques together is itself relatively new. Such a program should strive to ensure that completed inventories not only include high quality emissions estimates but also that those estimates are applicable and reliable for the intended purpose of the programs they support.

As emissions verification programs are applied in additional emissions development programs, the strengths and weaknesses of traditional technologies and approaches will become well defined. Researchers should be aware of the weaknesses of common techniques and promote the application of innovative techniques and approaches to overcome these weaknesses. New computer systems and mathematical analyses should be considered in all coordinated verification efforts. Examples of systems include Geographic Information Systems (GIS), statistical applications, graphic presentations, Monte Carlo simulations, and relational databases. Examples of innovative mathematical analyses that should be considered for emissions development and verification include fuzzy logic, artificial intelligence systems, chaos theory and fractal geometry.

DEFINITION OF TERMS

It is useful to define some key terms relative to the inventory verification process that will be used throughout the remainder of this report. Often individual inventory developers and/or inventory users will define these terms in the context of their own applications or goals. Therefore, the following definitions of key terms are provided to promote common usage in the context of this report.

Accuracy	Accuracy is a measure of the truth of a measurement or estimate. The term accuracy is often used to describe data quality objectives for inventory data, however, accuracy is hard to establish in inventory development efforts since the truth for any specific emission rate or emissions magnitude is rarely known.
Precision	The term precision is used to express the repeatability of multiple measurements of the same event. In experimental applications a measurement or measurement technique could have high precision but low accuracy. The term precision is also used to describe the exactness of a measurement. The term precision is not well suited for use in emissions inventory development.

Confidence The term confidence is used to represent trust in a measurement or estimate. Many of the activities discussed in this report are designed to increase the confidence that inventory developers and inventory users have in the databases. Having confidence in inventory estimates does not make those estimates accurate or precise, but will help to develop a consensus that the data can be applied to problem solving.

Reliability Reliability is trustworthiness, authenticity or consistency. In the context of emissions inventories reliability and confidence are closely linked. If the approaches and data sources used in an inventory development project are considered reliable, then users will have an acceptable degree of confidence in the emissions data developed from those techniques.

Quality Control Quality control activities are those procedures and tests that can be performed during the planning and development of an inventory to ensure that the data quality objectives are being met. These activities may include criteria tests for data on operations, completeness criteria, or averaging techniques for use in developing default parameters. Quality control activities are generally applied by the developers.

Quality Assurance Quality assurance describes the activities that are completed after the development of a product, usually by an independent party to verify that data quality objectives were met and that the product conforms to specifications. In experimental programs, audits with standard instruments and standard measures are used to establish the reliability of the experimental procedures. In emissions inventory development, however, few such standards exist. One effective activity discussed in this report is the use of an independent review team of experts to monitor the developments as progress is made on the inventory. The review team can identify alternate approaches and further documentation to enhance the credibility and reliability of the emissions estimates developed.

In the context of emissions inventory development, and in general use in this report, quality assurance is used to represent the sum of activities that are implemented to ensure the collection and presentation of high quality data.

Uncertainty Uncertainty is a statistical term that is used to represent the degree of accuracy and precision of data. It often expresses the range of possible values of a parameter or a measurement around a mean or preferred value.

In some applications involving emissions inventory preparation, it is possible to describe in statistical terms the relative accuracy of an estimate and ultimately provide a preferred estimate or central value and a percent range that bounds the actual value. Such opportunities are frequently limited to sources that have requirements for extensive monitoring, through continuous emissions monitors, to verify emissions rates. More often, however, the data that is available is insufficient to develop statistically based quantitative measures of the data accuracy. In these cases, subjective rating schemes are often used to describe the relative confidence that is associated with specific estimates.

In the context of this emissions verification report, uncertainty is used to represent any of several techniques or procedures that can be applied to establish a ranking or numerical scale to compare the reliability of and confidence in the emissions estimates. In their simplest forms, such ranking procedures are subjective evaluations that reflect the accuracy or reliability of estimates based on the opinion of the developer. In other applications the evaluation is guided to a specific attribute of the data. For example, the completeness, coverage, or specificity may be of special importance and developers may be asked to rate the final emissions estimates relative to one or more of these components that can affect the quality of the estimates.

Validation

Validation is the establishment of sound approach and foundation. The legal use of validation is to give an official confirmation or approval of an act or product. Validation is an alternate term for the concept of verification as used in this context.

Verification

The term verification is used to indicate truth or to confirm accuracy and is used in this report to represent the ultimate reliability, and credibility of the data reported.

In the context of this report verification refers to the collection of activities and procedures that can be followed during the planning and development, or after completion of an inventory that can help to establish the reliability of the inventory for the intended applications of that inventory. In this context, the representativeness of the final data for the intended applications is of more importance than the absolute accuracy of the final emissions estimates. The procedures identified as verification activities will be applied to establish confidence that the data are sufficient in terms of coverage, completeness and reliability to guide decision makers to effective policy options.

These verification approaches can be used to understand the strengths and weaknesses of completed inventories relative to the desired applications of the data. In this context, verification procedures should be useful in directing research to improve the underlying data or procedures used to develop emissions estimates in future programs.

Transparency — In the context of this report, transparency is used to represent the condition of being clear and free from pretense. The use of the term implies that data collected and reported by different agencies will be similar and, therefore, easily understood by other parties and comparable to the data presented by the other parties.

Compliance — Compliance is the act of conforming or yielding to a specified norm or protocol. In the inventory development process, compliance may indicate conformity to development protocols or international agreements. In this sense, the compliance issue can be thought of as verification that these established and agreed norms are achieved. The concepts of verification discussed in this report, however, are not intended to support the idea of compliance to norms or international protocol.

OBJECTIVES

This report is intended to provide a comprehensive summary of procedures and techniques that can be applied to emissions inventory development projects to help establish the accuracy and reliability of the emissions data for the intended applications of the inventory. The techniques discussed range from routine quality assurance activities that are a mandatory part of any technical effort to specific experimental and field measurement studies that can be applied to specific parts of inventories. Each of the techniques can be used independently or in combination to satisfy the demands for establishing credibility and relaiability of emissions data for essentially any purpose. The selection of the specific procedures that could be useful in any given inventory project are dictated by the intended applications of the project, the resources available for the development, and the time constraints. The objectives of this report are summarized below:

- Present a comprehensive list of possible methods for application to emissions inventory verification procedures.
- Provide examples of the application of these techniques from past projects or proposed technical applications.
- Document the background information for these techniques to provide a roadmap for users to obtain additional more specific information.
- Present a summary list of possible techniques associated with broad emissions source categories and to provide some guideance on the priority of these various techniques if resources and time constraints were not an issue.

ORGANIZATION OF THE REPORT

The report begins with an overall summary of the findings of the project. This section is organized in matrix format with broad categories of emissions verification approaches matched to broadly defined source categories. The matrix entried identify those procedures that have been applied or proposed for application for verification of emissions for sources in the indicated source categories.

The remainder of the report is organized to follow the approach agreed to by the Verification Expert Panel of the Task Force on Emissions Inventories commissioned by the UN/ECE. The five primary program elements listed below were identified in the preliminary meetings of the Verification Expert Panel.

- Documentation of Data Quality
- Application of the Data
- Comparison of Alternative Estimates
- Uncertainty Estimates
- Ground Truth Verification

Each of these program elements provides information that is useful to promote the development of high quality and representative emissions estimates. The information developed through these activities can be applied to establish confidence in the final inventory data. The information can also be applied in programs to establish comparability between different databases and to identify the strengths and weaknesses of the resulting inventory. The first two of these elements involve planning and coordination, and the last three represent specific activities that can be included in the overall inventory development and application programs. Specific activities that can be considered and implemented as components of emissions inventory development programs include comparisons of alternative estimates or estimation techniques, assessments of emissions uncertainty and reliability, and ground truth verification studies that rely primarily on field and laboratory measurement programs.

Documentation of data quality includes the development of a set of data quality objectives and criteria that will be applied to ensure that those objectives have been met. These efforts begin with the planning of the program and are directly related to the purpose of the study, the resources available to complete the study, and the schedule constraints imposed on the study. These activities require the definition of needs, criteria for accepting data sources, contingency plans for the use of backup approaches, and the definition of a quality assurance and quality control (QA/QC) protocol; activities may also include provisions for a third party review of the inventory development program and resulting inventories.

Considerations of the applications of the data and the needs of the inventory user community are the primary factors that control the requirements of any inventory development project. Often it is necessary to compromise based on the availability of data and other technical resources. Detailed planning and program flexibility are keys to the success of many inventory development programs. The applications of the inventory define parameters such as the geographic scope; the spatial, temporal, and species resolution of the databases that are to be generated in the program; and the approaches that can be implemented to achieve those needs. The types of program applications that influence inventory needs include source permitting and source-specific emissions increments, area-wide assessment studies to determine the relative magnitude of source category groups, air quality modeling analyses, source-receptor modeling analyses including relative VOC/NO_x and CO/NO_x ratios, and policy analyses to establish, implement, and track urban or regional control strategies.

Often multiple approaches can be applied to develop an emissions inventory. While the different approaches identified for any specific project may not always meet the statistical requirements that represent independent methods, it can generally be assumed that convergence of multiple approaches to a common emissions estimate contributes to the confidence that users have in the resulting inventory. Such analyses are also very useful in establishing priorities for any further efforts that are anticipated to improve second or third generation inventories. It is always desirable to establish ranges to represent the likely maximum and minimum emissions magnitude in addition to the mean or preferred estimate. These ranges can provide an assessment of the uncertainty or reliability of the emissions estimates. These analyses can assist in understanding the weaknesses of the resulting inventory and in interpreting the results of other technical- or policy-related applications using the inventory data. Emissions data are almost always based on estimates of at least one and often more than one critical parameter. Therefore, standard types of propagation of error analyses are normally not applicable to emissions data. It is possible in many cases, however, to provide reasoned bounds on the resulting inventory data. These types of analyses are particularly important for sensitivity studies associated with modeling applications. Sensitivity studies are used to determine the effect on control strategy conclusions for the different extremes represented in the inventory. Examples of these types of analyses will be discussed in more detail later.

The ideal emissions inventory would be based on direct measurement of all sources of interest in a program. This approach is obviously impossible in all but the smallest scale and most specific of cases. Therefore, verification of emissions estimates is sometimes related to comparison of the estimates with a small set of measurements or through some other innovative comparison technique. The Verification Expert Panel selected the term "ground truth verification" to represent these types of analyses. There are many opportunities for such analyses. Some examples that have been applied previously in programs in the United States, and some techniques that have been suggested for application to future programs will be discussed later in this report in some detail.

PRINCIPAL FINDINGS

This report is the culmination of an effort that has been ongoing for over two years. The concepts and techniques for emissions inventory verification discussed in this report have been developed through interactions with a large number of experts in air quality and emissions inventory studies from the United States and European countries. The ideas expressed here, therefore, cover a wide range of emissions verification opportunities including simple approaches and some rather sophisticated techniques that rely on emerging technologies.

The selection of the most appropriate technique or combination of techniques for application to any given inventory development project is dependent on several factors including the nature of the projects that the inventories are expected to support, the visibility of those projects, whether or not the projects involve cooperative efforts of several countries or other geopolitical entities, budgets and other resources available for the project, and schedule constraints. It is recognized that the more experimental and research oriented concepts discussed in this report will not be used in the majority of inventory development projects. Increases in the sophistication of modeling and data manipulation techniques, and the need for more detailed control strategies that target less traditional source categories, however, do suggest that more accurate and flexible emissions inventory data will be required in the future. Those future inventory development programs could benefit from the application of many of the approaches discussed in this report.

The advantages of high quality and accurate emissions data in air quality management projects is obvious, but it is perhaps more important to mention the disadvantages of using poor quality data with limited credibility. At the least, any inventory development project should include a comprehensive list of data quality objectives and criteria for evaluating the resulting inventory data against those objectives. It is also recommended to include as a minimum a simple data quality rating approach and to document the assumptions used to derive the qualitative ratings. Without such an analysis, the results of the inventory and the analyses that depend on the inventory can be questioned. Regulatory initiatives and policy options can be adversely affected if there is a general perception that the underlying data is incorrect or unreliable. Obviously, more rigorous statistical uncertainty and measurement based verification approaches are preferred and should be considered whenever they are possible. All inventory developers are also encouraged to share their experiences with emissions inventory verification approaches so that the wider emissions inventory community can benefit from those experiences.

The procedures and techniques discussed in this report are intended to support inventory development programs, and efforts that apply emissions inventory data to regulatory or policy making activities. It is possible to apply similar emissions inventory verification activities to demonstrate compliance with international protocol or agreements. Although this more universal application is not addressed specifically in this report, many of the principles outlined here could be used in such compliance demonstrations.

The most significant finding of this work is simply that there are many possible methods and techniques that can be applied to establish the reliability of emissions inventories and to help understand the weaknesses in inventories. This report presents many of these, although there are undoubtedly some techniques and methods that have been overlooked. The report presents examples of the application of some of these approaches to give inventory developers some ideas of how these approaches can be applied and the benefit that can be derived from including such procedures in their inventory development programs. To the extent possible work describing the approaches discussed has been referenced to assist users in locating additional information on the specific techniques and their application.

A summary of recommended emissions verification approaches is provided in Table 1. This summary is prepared in a matrix format, linked to the second level of detail represented in the Selected Nomenclature for Air Pollution (SNAP90) source category listings that have been adopted by the CORINAIR 1990 project and selected as an organization approach for use in the UN ECE guidebook. These broad categories should be familiar to any researchers interested in the development of emissions inventories and the matrix format provides for direct transfer to any particular distribution of source categories or sector descriptions associated with an emissions database.

This matrix addresses the priorities for the adoption of specific verification techniques in a general sense. It reflects those cases where specific inventory verification concepts have been applied or are proposed for application in actual programs. Although some approaches are more suited to particular source categories, nearly all of the approaches could be applied to any source category.

TABLE 1. EMISSIONS INVENTORY VERIFICATION APPROACHES BY SOURCE TYPE

SOURCE CATEGORY	VERIFICATION APPROACH							
	High Priority		Second Priority		Third Priority		Low Priority	
	DSS	SU	DQR	AE	SA	ISS	AM	AFA
PUBLIC POWER, COGENERATION AND DISTRICT HEATING PLANTS								
Public Power and Cogeneration Plants	X	X	X	X	X		X	X
District Heating Plants	X	X	X	X	X			X
COMMERCIAL, INSTITUTIONAL AND RESIDENTIAL COMBUSTION PLANTS								
Comm., Inst. and Res. Combustion	X		X	X	X			X
INDUSTRIAL COMBUSTION								
Combustion in Boilers, Gas Turbines, and Stationary Engines	X	X	X	X	X	X	X	X
Process Furnaces Without Contact	X		X	X	X			X
Processes With Contact	X		X	X				X
PRODUCTION PROCESSES								
Processes in Petroleum Industries	X	X	X	X	X	X	X	X
Processes in Iron and Steel Industries and Collieries	X	X	X	X	X			X
Processes in Non-Ferrous Metal Industries	X	X	X	X	X			X

DSS Direct Source Sampling
SU Statistical Uncertainty Estimate
DQR Data Quality Ratings
AE Alternate Estimates
SA Survey Analyses
ISS Indirect Source Sampling
AM Ambient Measurements
AFA Allocation Factor Assessments

TABLE 1. EMISSIONS INVENTORY VERIFICATION APPROACHES BY SOURCE TYPE (continued)

SOURCE CATEGORY	VERIFICATION APPROACH							
	High Priority		Second Priority		Third Priority		Low Priority	
	DSS	SU	DQR	AE	SA	ISS	AM	AFA
PRODUCTION PROCESSES (continued)								
Processes in Inorganic Chemical Industries	X		X	X	X	X	X	X
Processes in Organic Chemical Industries (bulk production)	X		X	X	X	X		X
Processes in Wood, Paper Pulp, Food and Drink Industries and Other Industries	X		X	X	X		X	X
Cooling Plants			X	X	X			X
EXTRACTION AND DISTRIBUTION OF FOSSIL FUELS								
Extraction and 1st Treatment of Solid Fossil Fuels			X	X	X	X		
Extraction, 1st Treatment and Loading of Liquid Fossil Fuels			X	X	X	X		
Extraction, 1st Treatment and Loading of Gaseous Fossil Fuels			X	X	X	X		
Liquid Fuel Distribution (except gasoline distribution)			X	X	X	X		X
Gasoline Distribution			X	X	X	X		X
Gas Distribution Networks			X	X	X	X	X	X

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TABLE 1. EMISSIONS INVENTORY VERIFICATION APPROACHES BY SOURCE TYPE (continued)

SOURCE CATEGORY	VERIFICATION APPROACH							
	High Priority		Second Priority		Third Priority		Low Priority	
	DSS	SU	DQR	AE	SA	ISS	AM	AFA
SOLVENT USE								
Paint Application	X		X	X	X	X		X
Degreasing and Dry Cleaning			X	X	X	X	X	X
Chemical Products Manufacturing or Processing	X	X	X	X	X	X	X	X
Other Use of Solvents and Related Activities			X	X	X	X	X	X
ROAD TRANSPORT								
Passenger Cars			X	X	X	X	X	X
Light Duty Vehicles < 3.5 t			X	X	X	X	X	X
Heavy Duty Vehicles > 3.5 t and Buses			X	X	X	X	X	X
Mopeds and Motorcycles < 50 cubic cm			X	X	X			X
Motorcycles > 50 cubic cm			X	X	X			X
Gasoline Evaporation From Vehicles			X	X	X	X	X	X

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TABLE 1. EMISSIONS INVENTORY VERIFICATION APPROACHES BY SOURCE TYPE (continued)

SOURCE CATEGORY	VERIFICATION APPROACH							
	High Priority		Second Priority		Third Priority		Low Priority	
	DSS	SU	DQR	AE	SA	ISS	AM	AFA
OTHER MOBILE SOURCES AND MACHINERY								
Off Road Vehicles and Machines			X	X	X	X	X	X
Railways			X	X	X			X
Inland Waterways			X	X	X			X
Maritime Activities			X	X	X			X
Airports (LTO cycle and ground activities)			X	X	X	X		X
WASTE TREATMENT AND DISPOSAL								
Wastewater Treatment			X	X	X	X	X	X
Waste Incineration	X	X	X	X	X		X	X
Sludge Spreading			X	X	X	X		
Land Filling	X		X	X	X	X	X	
Compost Production From Waste			X		X	X		
Biogas Production	X		X		X			

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TABLE 1. EMISSIONS INVENTORY VERIFICATION APPROACHES BY SOURCE TYPE (continued)

SOURCE CATEGORY	VERIFICATION APPROACH							
	High Priority		Second Priority		Third Priority		Low Priority	
	DSS	SU	DQR	AE	SA	ISS	AM	AFA
WASTE TREATMENT AND DISPOSAL (continued)								
Open Burning of Agricultural Wastes			X		X	X	X	
Latrines			X	X	X			
AGRICULTURE								
Cultures With Fertilizers (except animal manure)			X		X			
Cultures Without Fertilizers			X		X			
Stubble Burning			X		X	X	X	
Animal Breeding (enteric fermentation)			X	X	X			
Animal Breeding (excretion)			X	X	X			
NATURE								
Deciduous Forests			X			X		X
Coniferous Forests			X			X		X
Forest Fires			X		X	X	X	X

DSS Direct Source Sampling
SU Statistical Uncertainty Estimate
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AFA Allocation Factor Assessments

TABLE 1. EMISSIONS INVENTORY VERIFICATION APPROACHES BY SOURCE TYPE (continued)

SOURCE CATEGORY	VERIFICATION APPROACH							
	High Priority		Second Priority		Third Priority		Low Priority	
	DSS	SU	DQR	AE	SA	ISS	AM	AFA
NATURE (continued)								
Natural Grassland			X			X		X
Humid Zones (marches-swamps)			X			X		X
Waters			X			X		X
Animals			X		X	X		X
Volcanoes			X				X	X
Near Surface Deposits			X				X	
Humans			X					X

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DOCUMENTATION OF DATA QUALITY

The activities discussed in this section are related primarily to the planning stages of an inventory development program to ensure that the resulting inventory and quality assurance program applied to the inventory will be properly documented. These activities are completed to ensure that the finished inventory will be useful for the intended projects that depend on the inventory and to facilitate the application of the inventory in future programs. These records establish the strengths and weaknesses of the inventory and can be assessed at later times to determine whether the current inventory is suitable for other applications or whether major revisions or modifications are needed to support those additional programs. The major considerations discussed in this section include the following:

- Defining Data Quality Objectives
- Selecting Inventory Development Methods and Assumptions
- Defining Quality Assurance and Quality Control Procedures
- Defining Needs for Independent Review of Activities and Procedures

Activities associated with the documentation of data quality begin with the initial planning phases of any inventory development project and extend through the final production and documentation phase. The first step involved in these functions is to understand as completely as possible the needs of the users of the final inventories and to develop a set of data requirements and data quality objectives that are consistent with those needs. The remaining activities are included under the general heading of quality assurance. The inventory developers must establish the criteria, protocol, and data handling procedures that will be applied to the effort. Contingency plans are needed, to specify backup approaches, in the event that the primary approaches are found to be infeasible or ineffective. Quality assurance procedures should include a detailed plan for the review and acceptance of databases that are used in the inventory effort. Procedures for the correction or replacement of primary data inputs are required. All data applied in the inventory development should be documented with respect to their origin, date, coverage, and sponsoring agency. Finally, some programs may employ a separate outside committee to review the procedures and resulting databases. These additional reviews are very useful to establish credibility of the emissions estimates, the inventory preparation methodologies, and the inventory quality assurance activities. These review committees should be involved in the process from the initial inventory planning activities through the completion and documentation of the inventory development program.

ESTABLISH DATA QUALITY OBJECTIVES

Data quality objectives (DQOs) are defined as part of the initial planning phase of any inventory development project. The DQOs can be presented as a formal written component of the inventory research plan or developed informally through consideration of the project objectives. The DQOs specify the geographic scope, the spatial and temporal resolution, and the pollutant and source coverage, and, in some cases, the accuracy criteria to be applied to inventory components. The requirements for the accuracy of the inventory do not need to be specified in rigid quantitative or statistical terms as is common in laboratory experiments. Often it is desirable to define DQOs for emissions inventory programs in less stringent terms, to accommodate changes in the user objectives, and to respond to data weaknesses and other problems encountered during the inventory development project. Emissions data are estimates, and it is difficult to assign quantitative error bounds on these estimates; therefore, it is sometimes inappropriate to define quantitative error bounds in the development of DQOs.

The primary purpose of DQOs is to guide the inventory development team in the completion of a final inventory database that will fill the needs of the intended user community. This procedure requires a detailed understanding of the intended applications of the inventory. The development of DQOs is also influenced by the resources and time constraints of the inventory program. In some cases, some of the needs of the user community may not be achievable. In these cases, coordination and cooperation between the inventory development team and the intended users is required to agree on compromises and other procedures to ensure the best possible inventory to support the application program.

The experience obtained through the development of the 1985 NAPAP Emissions Inventory is used as an example of setting DQOs. The NAPAP inventory development effort was the largest and most demanding international inventory program ever completed. The inventory includes all emissions sources in the 48 contiguous United States and the ten Canadian provinces. Emissions were estimated for over 66,000 stationary point sources and for approximately 100 area source categories developed for each of the 3,057 counties in the United States and the 10 provinces of Canada. The inventory was resolved spatially to grid cells of 1/4 degree longitude by 1/6 degree latitude. Emissions data were allocated to represent hourly emission rates for the typical weekday, Saturday, and Sunday in each of the four seasons. Primary emissions species were resolved to represent 49 species classes for use in a variety of modeling activities. The final inventory was organized in over 100 files and consisted of well over one billion data elements.

Priorities were assigned to specific data elements as part of the DQOs developed for the 1985 NAPAP emissions inventory. These priorities are shown in Table 2.[2] This type of planning function serves as an example of how DQOs can be specified without using a strict quantitative format. Such priority assignments serve as a guide to the inventory development

TABLE 2. INVENTORY PRIORITIES AND DATA QUALITY OBJECTIVES FOR THE 1985 NAPAP INVENTORY

Data Record Parameter		Category I Plants[a]	Category II Plants[b]
State Data Submittal		H	M
Emissions Estimates	SO_2	H	1
	NO_x	H	1
	VOC	H	2
	TSP	M	M
	CO	L	L
Source Classification Code		H	H
Control Equipment/Efficiency		H	1
Operating Rate Data		H	1
Location Data		H	M
Stack Parameters		3	L
Temporal Operating Data		H	M
Other Key Data		M	L
Plant Confirmation of Data		4	L
Standard Industrial Classification Code		L	L

Key for Table 2.
- a Category I Plants Emissions Magnitude >500 TPY VOC; >1000 TPY for Other Pollutants
- b Category II Plants Emissions > 100 TPY for all Pollutants
- 1 High Priority for Combustion Sources; Medium for Other Sources
- 2 High Priority for Petroleum Refineries and Chemical Production; Medium for Other Sources
- 3 High Priority for Stacks > 100 feet; Low for Stacks < 100 feet
- 4 High Priority for Plants with Emissions of SO_2 and NO_x > 2500 TPY

team and help to ensure that the appropriate level of effort is allocated to each part of the inventory. The priority assignment also served as a reference for the users so that they knew what information would be available in the completed inventory. Changing needs and expanded applications of the inventory were identified during the NAPAP inventory development effort. As a result, some analyses using the NAPAP inventory data were affected by data weaknesses, even though the priority data elements were defined in the initial planning with input from both the inventory development and user teams. This condition is emphasized here to point out the need to build as much flexibility as possible into the inventory development process. In high visibility programs, such as the NAPAP effort, it is very likely that increased demands on the inventory will be requested after the initial planning is complete.

METHODS AND ASSUMPTIONS

Another important part of the inventory development planning process is to specify the methods to be applied to data collection and data processing, which in turn requires definition of the criteria to be applied to assess the various data sources that are available. These criteria are then used to make acceptance and rejection decisions for the various data suggested for application to the inventory. The criteria should cover the completeness of the data, the geographic scope of the data, the year of record for the data, the sponsoring agency that was responsible for developing the database, and the accuracy of the data, if known.

To the extent possible, consistency of data sources is desirable. The use of consistent databases for all similar sources in a region will facilitate inventory updates, projections to future years, and evaluation of alternative control strategies. It is sometimes possible to mix data sources in the development of a regional scale inventory. As an example, detailed traffic flow data may be available for an urban area through an urban transportation planning program, but traffic count or traffic flow data for the outlying suburban and rural areas may not be available. In many urban areas, the bulk of the mobile source emissions that affect the understanding of the problem and the design of control strategies would be included in the urban transportation planning area. Under these circumstances, it may be acceptable to use the detailed urban area data in combination with other simple estimates of vehicle traffic for the outlying area.

The issue of consistency is particularly important in programs that require inventories that cross country borders. Data consistency between countries is, however, sometimes very difficult to achieve. This may be particularly true in Europe, where recent political events have changed the communication and accessibility between countries, and in some cases, have changed the countries themselves. When significantly different emissions estimation techniques are applied in bordering countries, large discontinuities can result at the border. Such discontinuities can not only interfere with control strategy development and implementation, they can also affect the performance of air quality models. When planning an emissions inventory for a regional program that includes multiple countries, the consistency issue should be considered and common estimation methodologies should be applied whenever possible.

One useful approach to document inventory strengths and weaknesses is to implement a data quality rating scheme for emission factors and other supporting data that are to be used in the inventories. This approach has been advocated and implemented in inventory development activities in the United States. The U.S. EPA includes data quality rating factors to indicate the confidence in the emission factors that are listed in *AP-42*.

The data quality rating factors used in *AP-42* are specified as A, B, C, D, and E with A representing the highest quality and E representing the lowest quality. Although these quality ratings are rather subjective, they do provide an assessment of the confidence that can be associated with those factors. For example, these ratings were applied to the NAPAP inventory to establish the distribution of emissions by emission factor quality rating. These results are summarized in Table 3. In this example, it is clear that the confidence in the emissions for SO_2 and NO_x is much higher than for the other pollutants.

It is also possible to develop more complex data quality rating systems for application to emissions inventories. Such a system would consider factors such as geographic and temporal resolution of emission factors and activity data, as well as the quality and quantity of measurements made in actual systems to derive a weighted numerical score that would be assigned to emissions estimates. The numerical score would then provide a semi-quantitative quality rating scale that could be used to compare the reliability of two or more independent estimates for the same pollutant and source category combination. One such rating scheme is being considered for application to an international database of greenhouse gas emissions. Although the specifics of the rating system have not yet been applied to any published emissions data, this type of system could be applied at both global and country specific scales for application to global inventory programs and to source specific processes in regional and urban inventory programs.[4]

TABLE 3. DISTRIBUTION OF EMISSIONS IN THE 1985 NAPAP EMISSIONS INVENTORY BY EMISSION FACTOR DATA QUALITY RATING

POLLUTANT	EMISSIONS TOTAL, TPY[a]	PERCENT OF EMISSIONS BY DATA QUALITY FACTOR					
		A	B	C	D	E	OTHER[b]
SO_2	10,593,049	95.3	1.6	0.3	0.1	0.9	1.8
NO_x	5,321,622	67.9	14.5	10.5	1.7	2.1	3.3
VOC	444,454	7.0	9.2	10.6	5.2	13.1	54.9
TSP	608,977	18.3	20.3	8.3	6.4	5.4	40.8
CO	1,945,290	17.5	10.5	18.8	0.4	16.0	36.8

[a] Total emissions estimated with emission factor files

[b] Unrated emission factor or use of an emission factor for a source category for which it is unrated

It is also important to prepare contingency plans and backup approaches that can be applied in the event that desired approaches do not provide adequate data, are not available within time constraints, or are incomplete or otherwise unacceptable. Contingency plans may involve the use of default values, surrogate factors, or other parameterizations to represent specific activities or source categories. It is desirable to define these contingency plans in the inventory planning phase and to involve the inventory users in the definition of the contingency plans.

QUALITY ASSURANCE AND QUALITY CONTROL PROCEDURES

A quality assurance plan is another important component of any emissions inventory development project. The QA plan provides the blueprint for all activities that are included in the program to ensure data quality and to achieve the particular objectives of the program. The QA plan specifies all of the activities discussed previously and the specific data checking and data correction steps that will be implemented during the preparation of the inventories. Many of the components of inventory verification that will be discussed in more detail in the remainder of this document are also activities that should be documented in the QA plan.

The QA plan specifies the types of data that will be collected, the procedures that will be applied to assess the applicability of those data to the program, the steps that will be taken to correct or modify questionable or incorrect data, the procedures for documenting data corrections or modifications, and the procedures that will be applied to process the data into formats that are consistent with the inventory applications. The QA plan must be consistent with the DQOs and the resources that are available.

The QA plan should include a well-defined corrective action plan and any specific procedures that are necessary to document what was done to substitute or modify the original databases. In most cases, it is useful to maintain a separate QA file. The file should be organized to allow simple and timely access to specific information concerning quality assurance activities performed on the data. One approach is an electronic audit trail. An audit trail file can be structured to facilitate review of information on the date of receipt of original data, the magnitude of the reported data, the type of QA problem associated with the data, the correction to that data, the date of the correction, and the person responsible for that correction. This type of file can allow a quick and comprehensive review of all data manipulations and corrections and can provide a format that allows the entire process to be archived so that analyses of these corrections can be completed long after the inventory development project is over. These electronic documentation techniques can be particularly useful if the inventory data are used in additional programs in the future.

Some specific QA activities that were applied to the 1985 NAPAP Emissions Inventory are the following:

- the definition of DQOs and priority data elements (see Table 2)
- completeness checks against previous inventories and follow-up to verify facility closures and start-ups
- checks that all high-priority data elements were included in data records
- checks that the data represented a consistent base year 1985
- checks of aggregate total emissions and operating data against alternative data sources (e.g., State and national fuel use data against data reported to the Department of Energy)
- internal consistency checks for specific sources to ensure that operating and emissions data were compatible
- an emissions confirmation by the facility for sources over 2,500 TPY of SO_2 and NO_x
- detailed computer and manual reviews of the 1,000 largest sources of SO_2, NO_x, and VOC
- maintenance of detailed and complete QA files for each State
- two separate mailings to the reporting agency with a request for correction or verification of questionable, missing, or incorrect data
- maintenance of a project docket containing references for all data sources and processing techniques used in the project
- maintenance of a computerized audit trail
- development and documentation of default values
- separate computer program elements to check the results after each phase of data processing
- computerized checks to ensure that all spatial, temporal, and species allocation files accounted for 100 percent of the input data
- identification of data records with inaccurate locations (data records outside of specified boundaries or over water bodies, etc.)
- complete and detailed series of reports documenting the inventory effort

INDEPENDENT THIRD PARTY REVIEW

If time and resources permit, an independent review panel or third party review can be useful for large, complex, and high visibility programs. It is useful for these review functions to be operative through the entire project, from planning phases through completion. The specific responsibilities of the review teams are to ensure that the proposed project will satisfy the objectives of the users, that resources are adequately applied to ensure the best product within time constraints, that QA objectives are reasonable and applicable, that activities conducted are consistent with the needs and DQOs of the program, that corrective actions are logical and appropriate, and that the documentation is reliable and clear. Written reports from the review team should be included in the overall QA files for the project. These written reports can be in the form of meeting minutes of regularly scheduled and *ad hoc* meetings or as a formal written report. After the final inventory is prepared, the review team should include an assessment of the overall effort that points out any deficiencies in the final product, but that also recognizes the strengths of the final product, in terms of whether the project adhered to plans, responded to the DQOs, and substantially fulfilled the needs of the project. During the development of the 1985 NAPAP Emissions Inventory, both an independent review panel and a third party review of the final inventory were employed. Both of these functions provided recommendations that resulted in improvements to the inventory.

APPLICATION OF THE DATA

The intended application of the completed inventory is the principal consideration when preparing and implementing an inventory verification exercise. The major uses of emissions inventory data and the specific needs for inventory verification programs related to each of these uses are discussed in this section. In some cases, it is possible to use data and analyses developed while conducting these activities for emissions verification exercises. Some examples of such opportunities are discussed in this section. The two primary uses of emissions data and emissions inventories are listed below:

- assessments of the specific air quality problems in an area and identification of the most important sources and source categories that influence those air quality problems
- input for regulatory activities including air quality modeling analyses and the design, implementation, and tracking of the effects of air quality control strategies

ASSESSMENT STUDIES

The requirements for specificity and accuracy of inventory data are less stringent for assessment studies than for the other applications of inventories. Top-down inventory development methodologies are usually suitable for application to assessment studies and annual emissions estimates for an entire industrial sector are often adequate for these purposes. Assessment studies. are generally intended to provide the background understanding of the primary causes of the air quality problems being evaluated. One example of an assessment type inventory is the preparation of annual trends inventories. In these applications, it is not necessary to develop estimates for specific source categories; it is usually more suitable to develop estimates for large industrial sectors such as electric power production and chemical manufacturing operations. Another example is an assessment study to define the ten largest source categories of VOC and NO_x emissions in an urban area. For both of these applications, total emissions of NO_x resulting from fuel combustion can be estimated from total energy demand estimates. In this type of study it would not be necessary to represent the emissions by boiler design or even fuel type. Similarly, total emissions of VOC, CO, and NO_x from mobile sources could be estimated from vehicle registration records, total regional fuel sales data, and assumptions about the fleet average fuel economy. Details about road type and speed classifications would not be required.

Alternative approaches for these highly aggregated estimates can sometimes be applied to add validity to the estimates if the emissions data developed through alternative approaches are comparable. In these cases, the detail required in the emissions estimates would not justify the use of a complex and detailed approach to emissions verification.

REGULATORY APPLICATIONS OF INVENTORIES

Regulatory activities are performed by air quality control agencies to define programs and policy options to reduce the negative impacts caused by air pollutants. The development of an air quality control policy usually uses an emissions inventory to estimate the potential for mitigating those problems and the costs that are associated with the control options. Some of the issues associated with regulatory activities that depend on emissions inventories are listed below:

- understanding the importance of local emissions relative to the impact of air contaminants that are transported from other regions
- understanding the importance of biogenic or other naturally occurring sources relative to the anthropogenic sources in an area
- establishing the relative importance of the various anthropogenic source categories to the overall controllable emissions burden

Air Quality Modeling Applications

The requirements for emissions inventories in air quality modeling applications, and the methodologies and activities required to validate these inventories are significantly more demanding than for assessment inventories. For application to air quality modeling programs, representative inventories of the appropriate species are needed at spatial and temporal scales consistent with the model formulation. It is necessary to develop the baseline inventory data at source-specific detail to represent the species, spatial, and temporal variability associated with the emissions. In the most complex modeling programs, the needs of the model community often change during the development of the inventory. It is important to build in flexibility to allow changes in program requirements to accommodate changing user needs.

An air quality model is a computer program that represents atmospheric transport, chemical reactions, and pollutant deposition phenomena as a collection of mathematical expressions. These models require meteorological and emissions input data and are used to simulate actual atmospheric conditions that result in air quality problems. Air quality problems such as urban ozone formation are influenced by local meteorological factors including wind speed, wind direction, temperature, and sunlight intensity. Since these factors are variable on hourly time scales, emissions data are also required at hourly time scales. The models used to simulate urban ozone formation are usually based on a mass balance approach in which pollutants are transported in response to the hourly behavior of the wind and temperature conditions. The models are structured to represent physical distance scales that can simulate the hourly changes. This spatial resolution is commonly represented by a regular grid pattern overlaid on the modeling region. Emissions data, therefore, must also be represented at these spatial and temporal scales to be compatible with the model formulation. Since emissions data are commonly estimated at the annual-level, and at country-, province-, or county-levels, techniques must be applied to convert the emissions estimates into the appropriate spatial and temporal resolution. VOC, NO_x, and particulate emissions data must also be resolved to represent the source specific chemical compounds included in the VOC, NO_x or particulate matter estimate, to adequately track the complex chemistry that occurs throughout an urban area. The following discussion provides information on the requirements of spatial, temporal, and species resolution of inventory data for modeling applications and provides some approaches that can be used to evaluate the quality of resolved inventory data.

Spatial Requirements for Modeling Applications

Emissions inventories used in urban and regional modeling studies require the most demanding specifications on any emissions inventories, because of the scope, range and level of detail needed. The verification needs for modeling inventories are dependent on the physical domain of the modeling exercise, the chemistry simulated by the model, and the specific regulatory applications that the model results will support. Specifically, the verification needs must address the data sources and methodologies applied to resolve the emissions data.

Spatial allocation refers to the development of spatially resolved emissions estimates consistent with the appropriate spatial scales of the model application. These requirements include both the physical location of the plant or source and the elevation at which emissions are released to the atmosphere through smoke stacks. Plant-specific location data are often available for large stationary point sources and, if such data are available, they can be used directly to locate those sources. Verification is sometimes accomplished by checking the physical location data or through mapping the data to identify sources that are inaccurately located. Misrepresented location data can place emissions points outside of the geographic domain of the study or over water bodies. Once inaccurate location data are discovered, they can be corrected by contacting representatives of the facility.

It is also necessary to represent the appropriate height of the emissions release for large point sources from elevated smoke stacks. The effective release height is defined as the stack height plus the plume rise, which is the vertical distance travelled by the emissions plume before the plume levels out and begins to disperse in response to the wind at that height. The plume rise is affected by the speed at which the emissions are released from the stack and by the buoyancy of the hot stack gas. Plume rise is a function of the stack height, stack mouth diameter, stack gas temperature, and volume flow rate of the stack gas. In some cases, these parameters are known and can be included in the data collection protocol. When these data are not known, it is necessary to apply default parameters to estimate the effective release height. Stack parameters are frequently checked in inventory applications by determining whether the parameters are outside of a typical range of values. For example, stack heights for large coal burning utility plants should not have stack heights lower than 200 feet or higher than 1250 feet. Similarly, stack diameters should be less than 20 percent of the reported stack height.

Commonly, mobile and other dispersed area sources are estimated at some aggregated level of spatial resolution (e.g., in the United States, these estimates are often made at the county level). The spatial processing of these data involves formatting the inventory data to represent a regular grid pattern. The appropriate scale is dependent on the particular modeling application. For urban air quality modeling, the grid pattern is usually on the order of one kilometer to five kilometer squares. For regional ozone, visibility, or acid deposition modeling, the scales can be expressed in kilometers or degrees of latitude and longitude. The patterns represented in these models can range from 10-kilometer to 150-kilometer squares or equivalent resolution expressed in units of latitude and longitude. Global models are usually represented by degrees of latitude and longitude and typically range from 0.5- degree to 10-degree cells.

The methodology used to spatially allocate emissions is to apply spatial allocation factors. The spatial allocation factors represent the fraction of the activity that is included in each grid that overlaps the area covered by the emissions estimate. Figure 1 illustrates this concept for an example case involving a single grid cell that overlaps three emissions regions, represented here as counties.[5] In this example the allocation is based on land area. The area units represented in this illustration are arbitrary but could represent any standard area measurement units. In the grid cell shown in Figure 1, emissions would be allocated in the following manner for all source categories that were linked to the example spatial factor:

$$
\begin{aligned}
\text{Total emissions in grid cell X} \quad = \quad & 0.119\ (6.37/54.1) * \text{emissions for County A} \\
+ \ & 0.032\ (1.58/48.8) * \text{emissions for County B} \\
+ \ & 0.053\ (2.81/52.5) * \text{emissions for County C}
\end{aligned}
$$

Similar functions that describe the proportion of overlap of the selected surrogate data are developed for all occurrences of county and grid cell overlap, so that all of the emissions in each

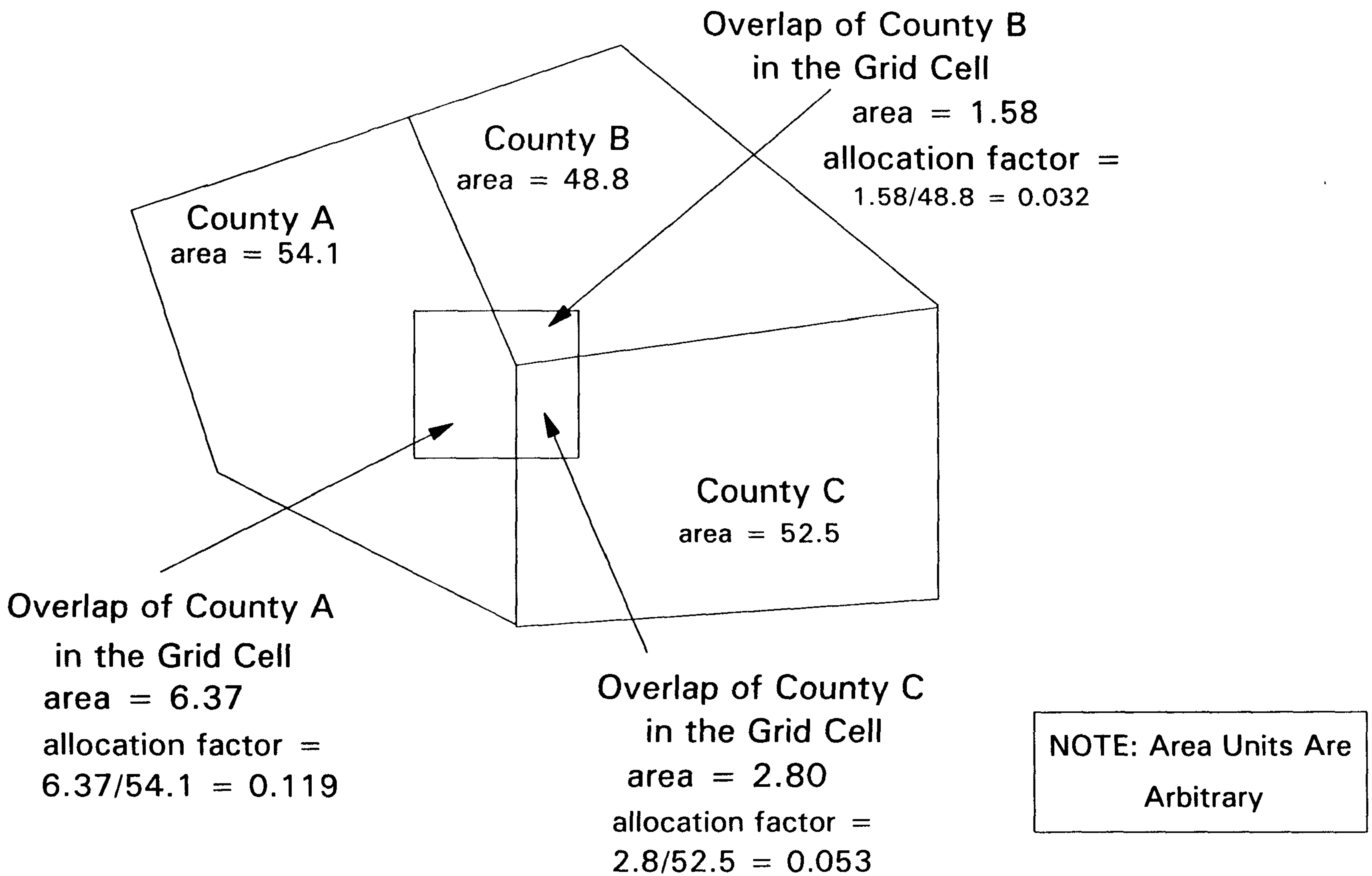

Figure 1. Example of County to Grid Cell Land Area Allocation

county are ultimately assigned to a grid cell. The development of these spatial factors requires the preparation of a separate spatially resolved data file for each spatial allocation factor and can be a costly component of the inventory development process. Some allocation factors can be developed from detailed census data, while others may require analysis of satellite imagery data. Therefore, the effort is usually limited to the preparation of a small set of factors that can be used to estimate the distribution of a large number of sources. For example, population and employment statistics for specific economic sectors are appropriate surrogates for many activities. Other useful factors are urban land area, agricultural land area, forested land area, and the area of water bodies.

The types of sources and source categories that require spatial processing depend on the scale of the modeling application. On urban scales, mobile sources, residential fuel combustion, pesticide application, road paving operations, and dry cleaning operations are examples of the activities that would be allocated using spatial factor files. Inventories prepared for extended regional modeling and for global modeling applications would likely use spatial allocation techniques for a larger number of sources than for urban modeling scales. The needs for source-specific location data become less important in larger scale modeling applications because the spatial averaging inherent in those larger scale models does not support the use specific location data. In the global applications, all sources can be estimated at national levels and spatially aggregated to the model grid resolution through the use of spatial allocation factors.

Geographic Information Systems (GIS) provide efficient spatial processing capabilities for application to emissions inventories. GIS programs are computerized data processing tools that are structured to facilitate mapping and distributing data in a spatial format. These programs allow the application of layers of data that can automatically be interrelated. It is necessary to construct spatially resolved surrogate data similar to those used in non-GIS spatial allocation techniques. The GIS programs, however, can overlay the spatial distribution data onto the emissions data and automatically calculate the allocation fractions, to conform to user-defined resolution. These approaches allow the user to produce several gridded emissions files at different scales using a single file of spatially resolved surrogate data. The use of GIS systems can, therefore, reduce the cost associated with spatial factor development if applications at different scales are anticipated. Any future emissions inventory development projects should consider the use of one of these GIS systems to simplify the application of emissions data in different modeling projects.

Temporal Requirements for Modeling Applications

Temporal allocation refers to the processing of inventory data prepared at annual resolution to represent seasonal, monthly, daily, or hourly fractions that are required by the models. Most manufacturing, utility, and service industries keep records of the level of activity conducted at individual facilities on at least an annual level. In many cases, detailed operating schedule data are available for the large stationary point sources. These data can then be processed through computer programs to represent data at the appropriate level of temporal resolution. In some cases, assumptions about continuous operation or a regular operating cycle provide fairly specific estimates about operating rates. These assumptions, however, do not always adequately represent variations in the efficiency of control equipment, process upsets, or accidental releases, and many times do not represent shutdowns for scheduled or unscheduled maintenance and repair activities. Therefore, assumptions about normal operating schedules can often add considerable uncertainty in temporally resolved emissions estimates, especially for application to an episodic simulation of an actual observed air quality event.

Typical temporal factors represent conditions of continuous operation: an eight-hour work day, five days per week, and a ten-hour work day, 6 days per week. While these assumptions about spatial and temporal allocation factors can be assumed to represent a large number of sources, the surrogate factors are not directly applicable to the distribution of any individual source category.

In the NAPAP application, annual emissions were resolved to represent hourly emissions, for the typical weekday, Saturday, and Sunday in each of the four seasons. This was accomplished by specifying seasonal fractions, days of the week in operation, and hours of the day in operation. The seasonal splits represented simply the fraction of the annual emissions that occur in each season. The days of the week operation data were processed to develop fractions for the weekday, Saturday, and Sunday. For example, a five-day work week schedule caused emissions to be equally distributed through all five weekdays and a six-day operating schedule allocated emissions equally to weekdays and Saturday. Hourly distributions were represented as typical work days. Typical assumptions included continuous operation with emissions distributed equally to each hour of the day and eight-hour operation with emissions equally distributed from 7 a.m. to 5 p.m. local time. Other more complex operating schedules were developed for application to highway vehicles, electric generating sources, and other source types that typically operate on irregular schedules.[6]

An example of using the application of the data as a verification tool is offered through the the experience of NAPAP. An analysis of daily emissions of CO was performed over the modeling region. It was discovered that emissions of CO in the grid cells surrounding New York City were higher on Saturday than on the weekdays. This was unexpected and further investigation revealed that emissions for pleasure craft were allocated spatially following the population distribution surrogate. Since it is expected that pleasure craft activity would be concentrated on weekends the emissions for this category were concentrated in high population density areas on Saturday leading to the higher CO emissions for New York City on Saturday. These types of analyses can be useful to understand the weaknesses of inventory data and to help with better interpretation of modeling and other analytical results.

Chemical Speciation Requirements for Modeling Applications

Species allocation involves representing the components of aggregated primary emissions species for modeling or risk determination applications. In the United States, emission factors represent the primary emission pollutants, namely SO_2, NO_x, VOC, PM-10, CO, and lead (Pb). In urban and regional ozone modeling, the components of the NO_x and VOC emissions are ultimately more important than the total NO_x or VOC estimate. Oxides of nitrogen include both NO and nitrogen dioxide (NO_2). Volatile organic compounds include literally hundreds of individual hydrocarbon compounds ranging from those that are only marginally active in urban photochemistry to those that are highly reactive. All air quality models used to simulate ambient ozone distributions represent the complex mix of VOC species as a group of representative hydrocarbon classes. The hydrocarbon classification involves either grouping compounds with similar reaction characteristics into a representative psuedo-species, or grouping similar carbon bond types that can be simulated by common reaction mechanisms. The degree of VOC grouping varies in various modeling analyses. The VOC species grouping approach and the number of representative VOC classes included in any modeling exercise is dependent on the specifics of the program and ultimately on the objectives of the analyses that use the modeling results. Estimation techniques based on source-specific profiles are often used to allocate the VOC source emissions estimate to the hydrocarbon classes that are required by the models. Similarly, source-specific allocation profiles are applied to represent the split between NO and NO_2. It is sometimes necessary to estimate size ranges for particulate emissions for application to visibility studies. Both VOC and particulate matter include individual compounds or elements that are considered hazardous air pollutants or air toxics. Modeling activities for risk assessments or other analyses involving the distribution of specific toxic compounds require inventories that have been speciated to represent those compounds of interest.

The speciation profiles represent the weight percent of the component hydrocarbons and elements included in the VOC and particulate emissions, respectively. The fractions were determined from source-specific emissions testing and subsequent laboratory analysis of the samples. There were a total of 313 specific hydrocarbon speciation profiles and 131 particulate speciation profiles applied in the NAPAP inventory. These profiles were applied to speciate emissions of VOC and particulate for well over 1,000 individual source categories of each pollutant.[7] Obviously, speciation profiles were applied to sources for which test results were not available. The assumptions about speciation characteristics can have significant influences on the chemistry represented in the air quality models, and the use of these surrogate speciation profiles adds large uncertainty to the modeling inventories. Since operating conditions vary even between sources that fit the same source category description, the use of a single speciation profile for all similar sources also adds unknown error to the emissions estimates.

Verification of Modeling Inventories

Air quality modeling teams are always interested in having a quantified error bound placed on the resulting hourly, gridded, and speciated emissions estimates. Each emissions allocation step adds uncertainty to the resulting emissions estimates, and it is almost impossible to quantify the error associated with the resolved estimates applied in modeling exercises. There are significant uncertainties in the model formulations themselves which are nearly impossible to evaluate without a clear understanding of the uncertainties in the model inputs. Specific activities that can be applied to modeling inventories to assist in estimating the validity of the emissions data will be discussed in later sections of this report.

If time and resources permit, it is sometimes possible to implement activities that can help to establish the reliability of the techniques used to resolve the inventories. In all cases, the data sources and the methodologies used to process these data into allocation factors should be documented and referenced. Such documentation can be helpful in evaluating the inherent validity of the raw data and the assumptions applied to process those data.

For the case of spatial allocation, estimates developed through the application of one allocation profile can be compared to the distribution that would result from another independent but related activity. For example, if mobile sources are allocated following a population surrogate, it is possible to compare that distribution to one based on traffic density estimates or a file of the distribution of roadways in an area. These types of checks generally do not provide quantitative error estimates, but they can often be useful to estimate the relative confidence that can be associated with a particular source category.

Checking temporal allocation profiles is not as straightforward as checking spatial allocation. If specific operating schedule data are available for some of the largest sources, it is possible to compare those data to the surrogate temporal profiles. These types of comparisons cannot provide quantitative assessments of uncertainty for other specific facilities, but they can often be used to provide a qualitative assessment of the reliability of those allocation factors. For example, in the NAPAP program, average operating schedule data were applied to many of the large coal burning utility sources as a default. Independent operating data were made available for the coal burning sources included in the Tennessee Valley Authority (TVA). The NAPAP operating schedules and the plant-specific operating schedules were compared, and it was found that the default operating schedule data were similar to the actual TVA operating data, in most cases. An example of one comparison of the various assumptions about hourly temporal allocation is shown in Figure 2. This result suggested that overall, the application of the temporal profiles representing the default operating schedules did not seriously affect the validity of the inventory. Not all comparisons were as good as that shown in Figure 2, and there was significant error for some particular sources. Figure 2 also shows the error that can result when continuous operation assumptions are used. In particular, routine and unscheduled shutdowns for maintenance and repairs are not represented by average or default operating schedule data. The effects of neglecting shutdowns of major coal burning utility sources were tested in sensitivity analyses using the Regional Acid Deposition Model (RADM) in the NAPAP program. These tests revealed that these types of shutdowns could seriously affect model results. Since the effects of facility shutdowns were so serious, and the temporal allocation methodologies did not accurately represent such occurrences, actual emissions data were represented for the largest 100 sources of SO_2 in the RADM modeling domain. A program was established to collect hourly emissions data from those sources that operated continuous emissions monitors (CEMs). Facility load and other operating data were collected for those sources that did not have CEMs, and hourly emissions were calculated. The detailed data were substituted for the average emissions data for modeling applications of episodic events in the NAPAP program.

Checking of speciation allocation methodologies is difficult. The only effective way to check the assumptions inherent in the speciation profiles is to conduct source tests and compare the results of the test to the speciation profile. Obviously, if all of the important sources are tested, there is no need for the application of the surrogate profiles. Even if selected sources can be tested, the tests themselves are limited by the selection of the individual compounds that are measured. One technique applied in programs in the United States is the evaluation of the speciation profiles quality and the assignment of a quality rating factor to those profiles as they are applied to individual source categories. It is then possible to assess the distribution of the resulting speciated data following the rating scheme. If a large fraction of the important compounds is associated with low quality ratings, the validity of the data can be considered suspect. Other techniques that involve comparisons to ambient measurement data are possible and will be discussed later in this report.

In all cases when allocation profiles are applied, the allocation profiles should be checked to ensure that they sum to unity. This will at least verify that the application of the profiles will not result in the loss or addition of emissions during the processing. It is also useful to check the emissions sums after each step in the processing to verify that the computer programs used in the allocation steps function correctly and do not result in changing the emissions estimates relative to the totals developed at the more aggregated level.

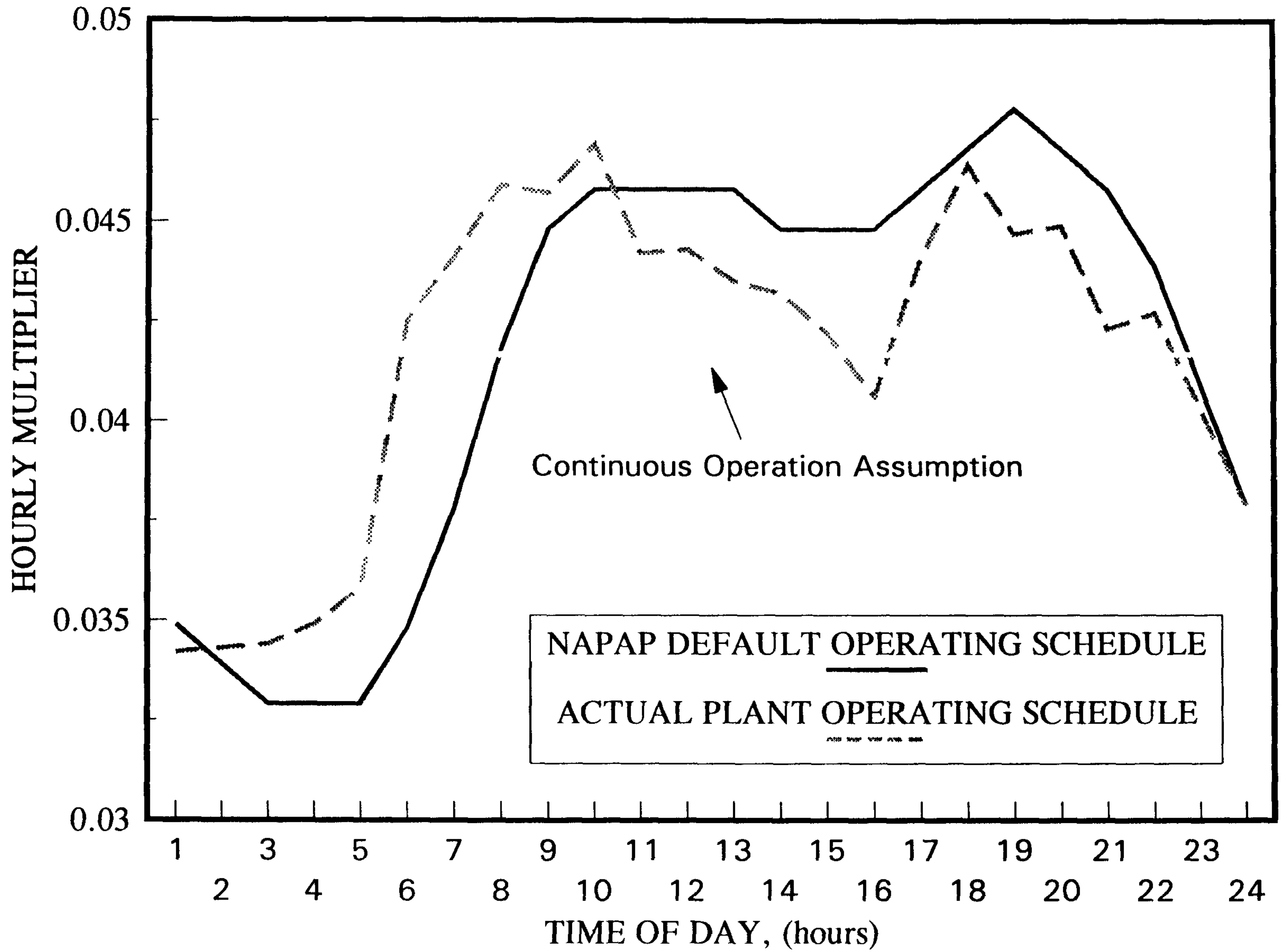

Figure 2. Comparison of Hourly Allocation Factors For An Actual Electric Utility Boiler

Control Strategy Analyses

Regulatory analyses are applied to all pollutants and at all scales. The analyses usually involve the identification and rank ordering of the sources or source categories as they are believed to affect the air quality problem under study. For example, a regulatory assessment of an urban ozone issue would seek to estimate the contribution of NO_x and VOC emissions from mobile sources relative to the magnitude of emissions from other fuel combustion, manufacturing, and service related activities. An additional component would be estimating the contribution of forests and other naturally occurring biomass to the total VOC emissions.

These types of activities are needed to estimate the total amount of emissions control that can be achieved and to provide preliminary control cost estimates. If an upwind location contributes to the local air quality problem, the regulatory agency may need to initiate discussions with their colleagues in the upwind area to quantify improvements that can be expected from their control programs. Similarly, if the assessment indicates that more than 50 percent of the ozone precursor emissions affecting an urban area ozone problem result from local mobile sources, the air quality decision makers should seek alternatives that could be adopted to improve public transportation or otherwise reduce the amount of personal automobile traffic.

Since these types of studies are used to better understand the principal issues and to develop policy planning approaches, the emissions data do not need to be highly resolved. Emissions data for these applications can often be developed using top-down approaches based on gross statistics such as fuel sales or even on population and economic statistics in some cases. Obviously, the level of detail required and the confidence associated with the absolute emissions estimates are not as rigorous as for other scientific and engineering studies. Often verification exercises can be implemented in which comparisons of per capita or other aggregated emissions estimates are compared to similar regions or even to other countries that have similar population density and economic development status.

Following the formulation of an initial policy based on the assessment, more detailed emissions estimates for the baseline case are required. These more detailed emissions estimates should be developed for specific types of sources that are targeted for control. One approach widely used in the United States is to characterize an industry as a series of model plants. These model plants can be differentiated by size and/or operating characteristics. The estimates of emissions rates for these model plants are developed through a detailed engineering study of the processes employed in the industry and a sound understanding of the causes of air emissions. Once these issues are defined, it is possible to evaluate the potential for add-on emissions control devices, changes in the operations, or other modifications, such as pollution prevention activities or recycling opportunities that could reduce air emissions. The costs associated with each of these options can then be evaluated, and cost benefit analyses can be developed. Decision makers can then assess the costs to society of the various options and the expected improvements in air quality that would result from the implementation of those activities.

Often the effects of a control strategy based on a collection of emissions control options are evaluated through the application of air quality models. Therefore, the needs for verification of emissions inventory data and the techniques that can be applied are similar to those discussed previously. Of primary concern in evaluating the impacts of control strategies is whether the range of emissions magnitudes associated with the uncertainty in emissions estimates leads to a similar decision about a proposed control strategy. Inventories that are bounded by ranges large enough to result in different policy decisions are difficult to apply in the regulatory framework. For example, if there are large ranges in emissions estimates associated with NO_x and VOC in an urban area, it is possible that the models would predict control strategies based on NO_x control at one extreme and VOC control at the other extreme.

Once the primary sources for control are understood and a cost-effective control strategy is proposed, the policy analyses must consider the implementation and tracking of the control program. The first consideration of emissions data used in this way is the need to develop projection inventories to represent the conditions likely to be encountered in the future. All control programs take time to implement, and changing populations, economic development, and new industrial activities all affect the future emissions scenarios. The development of verification techniques should consider not only the application to the baseline inventory but to the historical and the assumed future conditions as well. The success of control programs can then be evaluated against the expected range of uncontrolled and controlled emissions represented in the future year emissions projections.

Verification of Inventories for Regulatory Applications

The level of detail required in inventories used in regulatory activities is similar to that needed for modeling activities. Therefore, the activities suitable for verification are also similar. One approach introduced in the United States, with passage of the Clean Air Act Amendments of 1990, is to require each facility that emits more than 25 tons of a pollutant per year to report its emissions to the regulatory agency and ultimately to the U.S. EPA. The methodologies and data used by the facilities to estimate emissions must be documented to the satisfaction of the regulatory agency. These data will become a primary source of information to verify inventory estimation techniques and to improve existing inventories.

RELATIONSHIPS TO AMBIENT DATA

One of the primary indications of the potential inadequacies of ozone precursor emissions estimation methodologies is the apparent lack of agreement between VOC and NO_x concentrations, the VOC to NO_x ratios (VOC/NO_x), and CO to NO_x ratios (CO/NO_x) represented in emissions inventories and those measured in urban atmospheres. Ambient air measurement programs have long been a tool for assessing the air quality conditions in a location. Early morning VOC and NO_x concentrations are often measured in and near the urban centers as part of ambient measurements programs. These early morning measurements in urban centers are designed to provide emissions data during the period of high density morning traffic (6 to 9 a.m. local time), before significant chemical reaction has a chance to change the hydrocarbon and NO_x concentrations. The ambient measurements are then used to initialize air quality models in terms of VOC and NO_x concentration and the associated VOC/NO_x ratio.

The predictions of complex air quality models that simulate the interactions between all sources in the urban area over multiple days often do not simulate the measured VOC/NO_x ratios in the urban center. Much of the cause for the failure of the models to simulate these ratios has been attributed to inadequacies of the emissions input data. A recent study conducted by the California Air Resources Board (CARB) has presented detailed analyses of the application of comparisons of measured VOC/NO_x and CO/NO_x to evaluate the weaknesses in emissions inventories in the Los Angeles area.[8] The study design attempted to relate the measured abundance of VOC and CO to the amount of VOC and CO that would be expected from the highway mobile source categories in the inventory. The results found that the emissions models used to estimate mobile source emissions underestimate CO emissions by a factor of about 2.7 and underestimate VOC emissions by a factor of about 3.8. These and other measurements studies[9,10] suggest that much of the discrepancy may result from the treatment of a small percentage of high emitters as if they had emissions characteristics similar to the average test vehicle. The results of this program will be discussed in more detail in the section of this report covering ground truth verification methods.

The results of these and other studies suggest the current methodologies for inventory preparation do not consider all of the factors that are important in episodic analyses. While the current methodologies do seem to do a good job of estimating emissions at national levels and for annual time periods, there is a need to improve existing and develop new methodologies for temporally resolved, area-specific emissions estimates. Further application of data from programs comparing ambient measurement data to emissions inventory data will help to identify those sources and source categories that need improved emissions estimation methodologies and those that are missing altogether from the inventory preparation process. In the United States, additional programs are ongoing to identify and develop estimation methodologies for source categories that have not been included in previous inventory development efforts.[11]

COMPARISON OF ALTERNATE ESTIMATES

It has already been mentioned that alternate approaches exist for estimating emissions magnitudes from selected source categories. These alternate approaches can be used to derive independent estimates of emissions. The validity of the data resulting from two or more independent emissions estimates can be inferred from the degree of agreement among the estimates. Some examples of such data comparisons are discussed in this section. While some opportunities for data comparisons require extensive efforts in deriving alternate estimates, others require only a limited additional resources. This discussion will focus on the simpler kinds of data comparisons, which will be most useful in the widest range of applications.

OPPORTUNITIES FOR DATA COMPARISONS

Opportunities for data comparisons exist on many levels. It is possible to compare alternate emission factors, alternate operating rate data, and the final calculated emissions based on independent methodologies. Statistical comparisons of aggregate emissions totals may be applied between countries or regions of countries that have similar population and economic status. In each of these cases, the convergence of estimates derived through alternate estimation strategies adds credibility and validity to the final reported estimates.

One of the first data comparison opportunities in any inventory development effort is a completeness check. A completeness check involves a comparison of the facilities included in the current inventory to those included in previous inventories, if a recent emissions database is available. Completeness checks ensure that all of the important source categories are considered in the inventory, and that all of the facilities within a source category are included. If individual facilities are represented in the base line inventory, all of the significant sources of the pollutants of interest can be compared to the sources included in the previous inventory. In an area with a dynamic economy, some sources may no longer be in operation or new sources may have been added since the earlier inventory was developed. Records of the parent company or records maintained by trade associations can be checked to determine whether sources were closed or started up in the area. Where a discrepancy between the sources in two inventories is discovered, the inventory development team should seek to verify whether a source was actually closed or a new source was started.

In some cases, the inventory developers may encourage the application of source-specific emission factors, in lieu of the default or otherwise recommended factors, if sufficient documentation of the source-specific emission factors can be provided. The agency or authority responsible for the development of the inventory should review all source-specific emission factors to assess their applicability in relation to their quality and consistency with the rest of the inventory. In general, source-specific emission factors, for well-characterized sources, should agree to within about 20 percent of default or otherwise recommended factors. If the discrepancy is larger, the data upon which the specific emission factor is based should be reviewed. If the documentation of the development of the factors is unclear or otherwise inadequate, application of standard factors should be considered. In some cases, the revised factor could be based on actual emissions, and the default based on uncontrolled emissions. When uncontrolled emission factors are used, the predicted emissions magnitude must be corrected for the effect of the control equipment. In these cases, the comparison of final calculated emissions would be more appropriate than the comparison of the emission factors themselves.

Emissions estimates for major source categories at the country or regional level through two alternate measures of the inherent activity can often be developed. For example, emissions estimates for some manufacturing industries can be based on raw material feed to the process or on the total amount of product produced. Similarly, estimates of total gasoline fuel sales can be compared to the predicted vehicle miles travelled adjusted for the average vehicle fleet fuel economy to provide an assessment of the activity associated with motor vehicle use. Many of these types of comparisons can be facilitated through the use of graphical or regression analyses. An emissions inventory project should include as many of these simple comparisons as possible. An agreement among these comparisons can add confidence in the final emissions calculation without a large investment of resources or time.

In many cases, comparisons of alternate methodologies involve the comparison of a top-down methodology to a bottom-up methodology. The concept of top-down and bottom-up approaches has been introduced earlier in this report. Basically, a top-down methodology uses a country-level or some other aggregate estimate of an inherent activity and an average emission factor representative of the aggregate activity. Conversely, bottom-up approaches are based on the additive emissions resulting from specific conditions and operating characteristics of the population of specific facilities included in the source category. When the preferred inventory development methodology is based on a bottom-up approach, it is often possible to develop an estimate using a top-down approach quickly and efficiently. In such cases, the two emissions estimates can be compared, again without the expenditure of significant resources or time. For example, the national-level sales of a particular solvent could be compared to the source-specific estimates of the emissions of that solvent corrected for the amount of the solvent that is recycled or otherwise reclaimed.

Another type of comparison is based on the average emissions rate or emissions density, which can then be compared to the sum of source-specific emissions estimates for the population of facilities in a given source category. These comparisons are most valuable when applied to suorce categories that are comprised of a large number of small sources. An example of this type of comparison is an estimate of solvent emissions from dry cleaning operations expressed as a per capita rate, which can be compared to the emissions magnitude derived from records of the amount of dry cleaning fluids purchased by all of the dry cleaners in an area. Other opportunities for these types of comparisons include aggregate emissions expressed on a per-employee basis or on a per-square kilometer basis. These types of comparisons can be particularly useful in a country with little experience in inventory development. It is often possible to compare an aggregate average per-capita, per-employee, or per-area emissions density to similarly expressed emissions for a nearby country of similar economic status. Comparisons of aggregate emissions densities among countries can be particularly useful in Europe. In general, newly emerging nations and existing nations that have only recently moved toward cooperation in international environmental planning do not have well- established environmental programs. Resource and time constraints may make it difficult for such nations to develop comparison databases internally. Opportunities for comparison of emissions inventory data with other nearby countries with more experience in environmental programs and emissions inventory development may represent the only credible way of assessing the accuracy of these countries' emissions estimates.

Data comparisons based on control totals refer to comparisons of aggregate emissions and/or activity data to some other independent assessment of the aggregate emissions. The most common of these types of comparisons involves the comparison of the total emissions developed through a detailed emissions inventory program to aggregate estimates of emissions completed for a trend analysis. A trend analysis commonly relies on economic or industrial statistics that are published by government agencies. These statistics are generally developed for economic analyses and are often prepared at levels of aggregation that are not consistent with source categories used to develop emissions inventories. They are sometimes useful to provide a general assessment of annual emissions with the expenditure of modest resources. These approaches can be applied to historical records and to projections of the various economic parameters to estimate historical and projection inventories on the same basis as that for the current year. These analyses are useful in assessing the impact of control programs and the expected impact of future control programs that are under consideration by the regulatory authorities. While comparisons of detailed source-specific emissions estimates cannot be expected to match exactly with the aggregate trends types of analyses, reasonable agreement should be expected. Comparisons based on these types of analyses can be useful to point out large uncertainties or inadequacies in the detailed emissions inventories.

In applications involving the development of emissions control strategies, data on the extent and effect of existing control measures are also important. In the United States emissions data are often represented as uncontrolled emissions and additional information on control practices and control efficiencies are included as part of facility records. These control efficiency estimates can then be applied to the uncontrolled emissions to represent actual emissions. It is important to check the internal consistency of the individual source records to ensure that the assumptions about control devices and typical operating control efficiencies are reasonable. The concept of internal record consistency checks has been discussed previously. These checks are performed to verify that operating rate data are represented in the proper units, that control equipment has been identified correctly, and that stated control efficiencies are in the range expected for that control equipment type. These data can also be checked against similar operating and control device information for neighboring or nearby countries with a similar history of air pollution control. A summary of the types of comparisons involving emissions estimates and supporting data used in the development of emissions inventories is presented in Table 4.

APPLICATION OF COMPARISON DATA

While comparisons based on alternate data sources and alternate emissions estimation methodologies provide valuable tests of the validity of emissions data, they do not in themselves prove the accuracy of emissions inventories. The only true test of the accuracy of emissions estimates is a detailed comparison of the emissions magnitudes developed through the estimation procedures with simultaneous emissions measurements or detailed materials balance procedures. Emissions measurements involve actual source testing methods. Detailed materials balances involve an analysis in which all of the material input to a system or process is accounted for as being either bound in the product; released to air, or water or in solid form; or recovered for off-site disposal or for recycle. Each of these procedures is expensive and time-consuming and can only be accomplished on a limited scale. Naturally, if source test data are available they provide an excellent opportunity to check the emissions estimation procedures for those sources that have measurement data.

Emissions comparisons that provide results that are in general agreement do offer credibility to the final reported emissions estimates, and these types of checks should be included in emissions inventory development projects whenever possible. In addition to providing data that can be used to establish the validity of emissions data in an existing inventory, these types of checks can be used to identify weaknesses and uncertainties in the databases or methodologies used to generate the emissions estimates. The data or methodology weaknesses identified in these comparison analyses can direct inventory researchers in the development of future research activities to improve upon those weaknesses.

The examples included in this discussion suggest some of the types of comparisons that can be completed. Many opportunities exist for these types of comparisons, and it should be noted

TABLE 4. SUMMARY OF DATA COMPARISON OPPORTUNITIES IN EMISSIONS INVENTORY APPLICATIONS

DATA COMPARISON TYPE	EXAMPLES
Alternate estimation methods	• Emissions magnitudes based on raw material feed versus product • Emissions magnitudes based on alternate measures of the inherent activity
Top-down versus bottom-up methodologies	• National- or regional-level estimates versus source-specific totals within source categories
Emission density comparisons	• Aggregate estimates for per-capita, per-employee or per-area compared to total emissions from all facilities in a source category • Aggregate emissions densities compared to similar estimates from other countries or regions
Emission factor comparisons	• Source-specific emission factors compared to default or average factors • Uncontrolled emission factors with average level of control to controlled emission factors • Emission factors based on alternate measures of the inherent activity
Control total comparisons	• National totals compared to sum of all source categories or facilities within source categories • Summed emissions totals from detailed inventories compared to national totals in trends analyses • National totals compared to national totals of nearby countries corrected for population and economic status
Completeness checks	• Comparison to earlier inventories to check that all significant sources are considered • Checks that all important source categories are considered • Checks that all important data elements are included for facility records
Consistency checks	• Internal consistency for facility data records • Consistency of methodology for source categories • Consistency of methodologies between countries in multiple country inventory development

that comparisons at any level of detail are valuable for inventory development programs. The opportunities available include comparisons of emission factors, activity data bases, and emissions magnitudes developed through alternate techniques. Care must be taken, however, to ensure that comparisons are done for sources and source categories that are indeed comparable. Factors related to climate, economic development status, and other external influences can affect the degree of comparability that is expected.

UNCERTAINTY ESTIMATES

Experimental measurement data are commonly reported as average or preferred values with an associated error bound expressed in either absolute or relative units. The standard techniques for estimating experimental uncertainty depend on the known accuracy and precision of the measurement methods employed in the experiments. Since the accuracy and precision specifications of the data elements associated with emissions estimates are rarely known, these standard approaches for developing uncertainty are, in general, not applicable. There is a need, however, for reporting quantitative error bounds associated with emissions estimates. Several studies have been completed over the past decade to explore approaches for arriving at reasonable estimates of the uncertainty associated with emissions estimates. Perhaps the best example of attempts to establish emissions credibility is represented by the experience with the 1985 NAPAP Emissions Inventory. The discussion presented in this section includes the procedures and analyses of emissions uncertainty presented in the State of Science and Technology (SOS/T) Report No. 1 on *Emissions Involved in Acidic Deposition Processes*, prepared as part of the documentation of the NAPAP program.[12] Several other approaches have also been proposed, some of which take issue with the methods used in the SOS/T Report. This report references a number of recent publications in which the uncertainty issues are discussed in more detail, and interested parties are encouraged to refer to these documents for further reading on the subject.

Uncertainty estimates for emissions data are important for assessing both the inherent uncertainty of the emissions estimates for individual facilities and the range of emissions magnitude represented by all sources in a study area. The uncertainty estimates for individual facilities are useful to understand the likely impacts of source- specific control options. Uncertainty associated with the collection of facilities in a source category description and in the complete inventory are useful to assess the overall quality of the emissions data and the relative quality of the aggregate estimates of specific pollutants relative to the other pollutants active in the air quality issues of concern. The issue of emissions data uncertainty continues to present a significant challenge in air quality management programs. While the statistical techniques discussed in this report are useful for application to well- characterized sources, they are often not applicable to many sources of air pollutant emissions. The understanding of the effects of the estimation assumptions on individual facilities and the effects of assumptions inherent in the emissions allocation procedures has not yet advanced to the point that allows routine statistical uncertainty analyses of completed inventories. Efforts to improve this situation are continuing.

Since statistically rigorous uncertainty analyses are often difficult to complete, a variety of data quality rating approaches have been used. These approaches all rely to some degree on subjective analyses by the developers. Most of these approaches use a letter grade to indicate the confidence that is associated with the estimates, similar to the A through E rating scheme used in AP-42. One additional semi-quantitative approach is being considered by the U.S. EPA. This technique, known as the Data Attribute Rating System (DARS), is being developed jointly by the Office of Research and Development of the U.S. EPA.[13] The goal of this development effort is to provide a consistent rating system that results in quantitative scores that can be applied in comparative analyses. The technique is intended to be useful in a wide range of inventory applications. Conceptually, DARS evaluates the attributes associated with emission factors and activity data and the reliability of those parameters for the intended applications. The details associated with DARS are described following the discussion of more traditional statistical uncertainty analyses.

CAUSES OF EMISSIONS UNCERTAINTY

The fundamental approach for estimating emissions data is based on the application of the algorithm or model represented in Equation 1:

$$E = (AF)*(EF)*(1\text{-}C\ eff)*(All\ Fac) \qquad (1)$$

where:

where:	E	=	Emissions estimate for the source
	AF	=	Activity factor for the source
	EF	=	Emission factor for the source
use	C eff	=	Fraction of emissions removed by a control device in at the source
	All Fac	=	Factors for spatial, temporal, or species allocation

The uncertainty in the emissions estimate results from the combined uncertainty in each of the factors on the right hand side of Equation 1. With the exception of the activity factor, each of these parameters is an estimate that is based on a small number of measurements and is then universally applied to all sources within a given source category. Even the activity data is often an estimate, although the inherent uncertainty of the activity data is frequently less than that for the other parameters.

The recommended values for emission factors and control efficiencies are often based on the mean of a limited number of measurements for a small sample of the sources included in a source category. Differences in operating characteristics, maintenance and repair procedures, and in some cases climate and local weather conditions can affect the actual emission factor and control efficiency as applied to individual sources. In general, the variability of these parameters is determined by assuming that the individual measurements used to establish the average emission factor or control efficiency are normally distributed. The assumed uncertainty in these parameters is then related to the standard deviation of the individual measurements about the mean value.

The uncertainty of activity or operating data for point sources that maintain records of the raw material feed or amount of product produced is generally low, since these facilities normally maintain accurate records of these parameters. The estimate of the mean and variation about that mean for some area and mobile sources are often established through an engineering assessment or through the use of a model, and the resulting variability of the activity data for these sources can be quite high. In general, rigorous estimates of the uncertainties in these parameters have not been developed.

The uncertainty of allocation factors is also often based on engineering assessments. In select cases, for large point sources estimates of the variability in the application of typical temporal allocation profiles can be assessed through analyses of actual operating rate data (e.g., Figure 2). Even when such analyses are available the application of those estimates to all other sources in a source category can result in additional unknown error. Spatial allocation of point sources is generally known with a great deal of accuracy from plant-specific location data. The spatial allocation of area and mobile sources, however, is normally accomplished by the application of spatial allocation surrogates that do not reflect the variability in those activities resulting from personal lifestyles or other external influences. Speciation allocation factors are the largest source of uncertainty in these applications, and only limited information is available to assess these uncertainties. In general, uncertainty estimates based on the techniques discussed later in this section have not been developed for highly resolved speciated inventories, because the information to complete these analyses is simply not available.

The variabilities in the parameters used in the emissions estimation algorithm (equation 1) are assumed to result from random errors in the application of mean values for individual sources. There is also the potential for systematic error or bias in the emissions estimates. Bias results when one of the parameters used in the emissions estimation algorithm is based on unrepresentative data or does not consider some essential component of the emissions process. For example, if an emission factor is developed from source test data that were collected under load conditions or at operating capacities that are not representative of the normal operating conditions, that emission factor may include a bias when applied to the normal operating conditions. The uncertainty in an emission factor, estimated by considering of the standard deviation of emissions rate measurements performed at 100 percent capacity, will not reflect the systematic under- or over-prediction that would result from a bias in the application of that emission factor at normal operating conditions at a lower capacity.

For mobile sources, biogenic sources, and other source categories that use an emissions model to predict emissions, the models often consider only the most important variables that contribute to the variability in emissions rates. For example, biogenic VOC emissions are often predicted in the United States with an algorithm that depends on air temperature and sunlight intensity. Those two parameters explain only about 50 percent of the variability in the measured emissions rates.[14] Neglecting the effect of the variables that contribute to the remaining variability may introduce an unknown bias into the emission factors applied to biomass sources. Bias in aggregate emissions estimates can also be caused by the failure to consider all of the sources or source categories that contribute emissions in an area. Systematic error in emissions estimates is difficult to predict and the effects of the bias introduced in emissions estimates as a result of systematic error can have significant effects on air quality analyses that rely on emissions inventories.

APPROACHES FOR ESTIMATING EMISSIONS UNCERTAINTY

A number of approaches can be taken in ascertaining the level of uncertainty in emissions estimates for a particular inventory. The approach chosen can be based upon knowledge of the data distribution characteristics and should include any assumptions used in performing the emission estimates. The methods used for collection of the data also need to be considered so that the sample variance can be computed correctly before determining an uncertainty value.

One common assumption made in analyzing uncertainty in emission inventories is that the data are normally distributed and that the factors used in estimating emissions are independent. These assumptions allow the use of standard statistical analyses to determine the mean, variance, standard deviation, and confidence intervals. This approach has been applied in the NAPAP analyses, and is discussed in detail in the NAPAP SOS/T Report No. 1. A summary of the technique is presented later in this section.

It has been argued that emission inventory data are not normally distributed and that the use of the same emission factor for many sources in a given source category negates the assumption of independence. These factors may limit the ability to calculate the uncertainty in emission inventory data. These issues have been discussed in some detail by Benkovitz and Oden[15]. The methods for calculating uncertainty for an emission source category using a sum of individual, site-specific emission estimates or using averaged emission factors for all sources were reviewed. The authors state that the use of emission estimates for individual source sites reduces uncertainty in almost all circumstances. The authors also acknowledge, however, that the use of such techniques are not appropriate for source categories where a limited amount of empirical data is available on which to calculate some of the statistics needed to perform these estimates of uncertainty (e.g., many area sources). The utility of such methods is limited to sources that are quite well characterized such as power plants. Assuming that the original data used to develop the averaged emission factor is available, and that the parameters being used in the emission estimate are independent and do not vary with time, equations developed in this paper could be used to estimate the mean square error (MSE) of the sum of emissions and the variances needed to estimate the uncertainty in the emission estimate.

In a second paper, Oden and Benkovitz investigate some of the assumptions commonly associated with uncertainty analyses.[16] Specifically, they explored the assumption that parameters used in estimating emissions are independent and that their values do not vary with time. Although these investigations have not verified the assumptions of independence or that these variables change significantly over time, the results imply that the factors do not contribute significantly to the bias of the estimation. The general conclusion was that the emission estimates based on these assumptions will be unbiased for a wide range of time series. They caution, however, that proper accounting of the emission estimation parameters is necessary to ensure that the base assumptions used in determining uncertainty are valid.

A second approach to determining uncertainty involves the use of statistical techniques that do not require an assumption of data that are normally distributed. Non-parametric analyses, also known as distribution-free methods can be performed without consideration of the underlying distribution. A third alternative involves completing a logarithmic transformation of the data to approximate a normal distribution and then applying standard statistical analyses to the transformed data. Both of these approaches are discussed in detail by Ferreiro and Cristobal[17]. Examples of the application of these procedures are presented in the following discussion.

Analysis of Uncertainty Assuming Normally-Distributed Data

One approach to estimating emissions uncertainty, based on the technique discussed in the NAPAP SOS/T Report No. 1, is outlined in the following paragraphs. Readers are encouraged to refer to the SOS/T report for more detail concerning this methodology.[12] The approach relies on simple statistics including the standard deviation, the coefficient of variation, and the 90 percent relative confidence interval. The standard deviation (S.D.) is a commonly used statistic that describes, quantitatively, the spread of data points in a population of measurement data. The coefficient of variation (C.V.) is a measure of the standard deviation relative to the mean value (i.e., C.V. = S.D./mean). The 90 percent relative confidence interval is used to define the limits that include 90 percent of all possible measurements in a population assuming that the distribution of the measurements is a normal distribution. In a normal distribution, 90 percent of the possible measurement values lie within a range bounded by ± 1.64 times the standard deviation.

In this approach, the mean and standard deviation are determined for each element of the emission estimation equation. For the example presented here, we assume that the emissions estimate is the simple product of the AF and the EF, or E = (AF)*(EF). The C.V.s associated with the activity factor and the emission factor are then calculated. The C.V.s are combined to determine the C.V. of the final emissions estimate by applying Equation 2.

$$(1 + (C.V.)^2_{emiss}) = (1 + (C.V.)^2_{AF}) * (1 + (C.V.)^2_{EF}) \quad (2)$$

The 90 percent relative confidence interval is then calculated for the final emissions estimate by Equation 3.

$$\text{90 percent RCI} = C.V._{emiss} * 1.64 \quad (3)$$

An example, derived from the NAPAP SOS/T Report No. 1, is summarized in Table 5.[12]

The 90 percent confidence interval can also be estimated for the sum of these two sources following similar procedures. The mean emissions for the sum of the two sources is 900. The standard deviation of that mean can be estimated from Equation 4.

$$(\text{S.D. [combined emissions]})^2 = (\text{S.D. [plant \#1]})^2 + (\text{S.D. [plant \#2]})^2 \quad (4)$$

The standard deviation estimated for the sum of the emissions from the two plants is then 79.16. This value gives a C.V. of 79.16/900, or 0.09. The 90 percent relative confidence interval is then 0.15, which yields a 90 percent confidence interval of 767 to 1033. The result gives a range for the 90 percent confidence interval that is less than the sum of the 90 percent confidence interval for the two individual sources. This result demonstrates the concept that the overall uncertainty decreases as the number of sources increases.

Similar analyses can be performed for emissions estimates from a collection of source categories. An analysis demonstrating this concept based on emissions estimates from the 1985 NAPAP Emissions Inventory is presented in Table 6. The C.V.s for the emissions categories listed in Table 5 were derived from previous work completed by Chun.[18] Two analyses representing a lower and upper limit of the variabilities of NO_x emissions from the utility, industrial combustion, and transportation sectors are represented. These C.V.s are based on the available data and the most reasonable assumptions and as such represent the best estimates at this time. These analyses have been applied to establish that the overall uncertainty in the NO_x emissions estimates for the 1985 NAPAP emissions inventory is between 6 and 11 percent. Similar statistical relationships were also provided for the SO_2 estimates in the NAPAP inventory, and the results indicate that the overall uncertainty in the annual SO_2 emissions estimates is between 4 and 9 percent. Unfortunately, similar analyses were not completed for the annual VOC

TABLE 5. EXAMPLE OF AN UNCERTAINTY CALCULATION

	PLANT # 1	PLANT # 2
ACTIVITY DATA		
MEAN	100.00	50.00
STANDARD DEVIATION	2.00	1.00
C.V.	0.02	0.02
EMISSION FACTOR		
MEAN	5.00	8.00
STANDARD DEVIATION	0.5	1.2
C.V.	0.10	0.15
EMISSIONS ESTIMATE		
MEAN	500.00	400.00
STANDARD DEVIATION	51.00	60.54
C.V.	0.10	0.15
90% RCI	0.16	0.25
90% CONFIDENCE INTERVAL	416 to 584	301 to 499

emissions estimates, because credible assumptions about the variability of the VOC emissions for the major emissions sectors have not been developed. The overall variability in VOC estimates is much larger that those determined for NO_x and SO_2. The procedure presented in Table 5 could be applied to VOC if valid C.V.s for the emissions estimates for the large VOC sources are developed. The development of valid C.V.s will require a significantly improved understanding of the errors associated with the application of surrogate allocation data, emission factors and control efficiencies, and the relationships between these factors that affect the independence assumption.

TABLE 6. UNCERTAINTY ESTIMATES FOR NO_x EMISSIONS IN THE 1985 NAPAP EMISSIONS INVENTORY

SOURCE CATEGORY	EMISSIONS Tg/year	C.V.	S.D.	$(S.D.)^2$	90% RCI	90% CONFIDENCE INTERVAL
Low Variability Case[a]						
Electric Utilities	6.09	0.07	0.43	0.182	0.11	5.42 to 6.76
Industrial Combustion	2.25	0.15	0.34	0.114	0.25	1.69 to 2.81
Industrial Process	0.84	0.25	0.21	0.044	0.41	0.50 to 1.18
Residential/Commercial	0.62	0.30	0.19	0.035	0.49	0.32 to 0.92
Transportation	8 03	0.02	0.16	0.026	0.03	7.79 to 8.27
All Other Sources	0.81	0.40	0.32	0.105	0.66	0.28 to 1.34
Total	18.64	0.04	0.71	0.505	0.06	17.52 to 19.76
High Variability Case[a]						
Electric Utilities	6.09	0.09	0.55	0.300	0.15	5.18 to 7.00
Industrial Combustion	2.25	0.20	0.45	0.203	0.33	1.51 to 2.99
Industrial Process	0.84	0.25	0.21	0.044	0.41	0.50 to 1.18
Residential/Commercial	0.62	0.30	0.19	0.035	0.49	0.32 to 0.92
Transportation	8 03	0.10	0.80	0.645	0.16	6.75 to 9.31
All Other Sources	0.81	0.40	0.32	0.105	0.66	0.28 to 1.34
Total	18.64	0.06	1.15	1.331	0.10	16.78 to 20.50

[a] The low and high variability cases reflect different assumptions about the variability of emissions from utility sources with low NO_x burners and from the industrial combustion and transportation sectors from Chun.

For the totals, the overall S.D. is calculated as the square root of the sum of the squares of the S.D.s of the individual entries. The overall C.V is calculated from the overall S.D., which is then applied to determine the 90% confidence interval.

C.V. = coefficient of variation; S D. = standard deviation; RCI = relative confidence interval

Another example of the application of uncertainty analyses has been presented by researchers at the TNO Institute of Environmental Sciences in The Netherlands.[19] This publication provides an excellent discussion of the sources of emissions uncertainty and the concept of propagation of errors in emissions inventory development applications. This report presents quantitative uncertainty estimates for NO_x emissions from on-road vehicle emissions and stationary combustion sources. The report recognizes the difficulties in developing quantitative uncertainty estimates for other sources of NO_x and nearly all sources of VOCs.

The TNO report presents an analysis of uncertainties or expected variabilities for the major factors (e.g., the miles travelled by specific vehicle categories, the emission factor for specific vehicle categories, combustion and fuel characteristics in stationary combustion sources, measurement instrument error, sampling errors, and compounded errors in scaling spot measurements to annual aggregation) that affect NO_x emissions from these two important categories. The results of the study indicate that the overall uncertainties associated with motor vehicle and stationary combustion sources of NO_x are 4 percent and 2.6 percent, respectively. These analyses suggest that the emissions inventory techniques applied to The Netherlands national inventory underestimate true NO_x emissions slightly and that those estimates contain an overall uncertainty of approximately 3.5 percent.

Analysis of Uncertainty Using Distribution-Free Methods

Ferreiro and Cristobal have reviewed the methods for performing analyses using non-parametric or distribution-free techniques in an overall discussion of statistical handling of emission inventory sampling and analyses.[17] The methods that use summary descriptive statistics to characterize the distribution of emissions related data are presented along with methods for identifying the median, lower and upper fourths, outlier cutoffs, and extreme values (outliers) are discussed in some detail. The techniques to calculate confidence limits for the sample estimates and the description of the sample structure are also given in this paper. In this paper, the authors concentrated on the statistical treatment of these parameters and did not present any applications of these techniques to existing inventory data. The interested reader should review the paper for details and formulations.

An example of the application of non-parametric statistics to actual data has been presented by Khalil.[20] The uncertainties associated with global budgets of several atmospheric trace gases were estimated using a method that relies only on the ranges of emission rates. A simple range estimate based on the preferred value and expected range for each major category of the inventory was compared with a 90 and 95 percent confidence limit on the ranges constructed statistically from the range of each component. The resulting calculation of a 90% confidence interval produces a narrower range of emissions than that derived through an additive analysis. The base assumption for this technique is that the probability that any value in a sample range is equally likely (uniform distribution) instead of being clustered around some sample mean. These analyses can produce more meaningful range estimates for assessment and sensitivity studies.

SENSITIVITY ANALYSES

The types of uncertainty analyses presented above for annual emissions estimates are useful to assess the credibility and validity of the emissions data and the emissions inventory development process. The application of the emissions data at the annual level are, however, limited. Many of the analyses that use the emissions data require the chemically speciated inventories resolved to appropriate temporal and spatial formats. Estimates of the 90 percent confidence intervals for the resolved emissions estimates are used by modelers to perform sensitivity studies. Sensitivity studies are used to test the model predictions over the likely range of emissions to determine if different results are obtained at the extremes of the emissions range. Ideally, the sensitivity of model predictions to emissions inputs would address the individual components that contribute to the variability of the emissions. These results would assist both modeling and inventory development researchers to target the most critical issues for further research and improvements. Unfortunately, the current state-of-the-science on emissions inventory development cannot support these types of analyses. For example, consider the case of an industrial process that uses a solvent-based metal degreasing operation. If fugitive emissions of the solvent are not included in the point source inventory, the spatial allocation methodology may incorrectly add all or part of the emissions to an inappropriate grid cell. If the degreasing process is conducted intermittently in batch-mode, the use of a standard eight-hour work day would result in emissions allocation to hours of the day when no emissions are present. If outdated data are used to specify the chemical formulation of the degreasing materials, the speciation profiles will generate specific chemicals that may not even be used at the plant. In these cases, the idea of means and C.V.s to describe the expected variability of the hourly emissions rate of a particular compound would be meaningless, in the context of the analyses presented above. It could be stated that the uncertainty of the emissions data is 100 percent of the specified value; however, these types of estimates are not very useful for application to model sensitivity studies.

DATA QUALITY RATING SYSTEMS

Emissions inventory estimates are often calculated as functions of process rates, manufacturing units, control technologies, and factors for spatial, temporal, and species allocation. Estimates of each of these parameters are often based on a small number of measurements and the estimate is then universally applied to all sources within a given source category. Differences in operating characteristics, maintenance and repair procedures, and in some cases climate and local weather conditions can affect the actual emission factor and control efficiency as applied to individual sources.

Spatial allocation of point sources is generally known with a great deal of accuracy from plant-specific location data, but the spatial allocation of area and mobile sources usually requires the application of spatial allocation surrogates that often do not reflect the variability in those activities resulting from personal lifestyles or other external influences. Similarly, surrogates of temporal operating characteristics are often applied to allocate emissions to seasonal, daily and hourly levels when specific operating data are not available. Species allocation factors are the largest source of uncertainty in these applications, and only limited information is available to assess these uncertainties. In general, uncertainty estimates based on the techniques discussed here have not been developed for highly resolved species inventories, because the information to complete these analyses is simply not available.

Therefore, a meaningful measure of the overall reliability of an emissions inventory can sometimes be developed by the application of a data rating scheme. Rating schemes can have different formats, but each sets up some arbitrary scale that is applied to score individual emissions estimates at the appropriate level of aggregation. Several rating schemes have been discussed in the context of the UN ECE Task Force. Each of the schemes is briefly summarized below.

The U.S. EPA has long used a rating system for its preferred emission factor listings included in its AP-42 document.[1] This technique uses a letter rating system of A through E to represent the confidence in emission factors from best to worst. In this system A factors are based on several measurements of a large number of sources, and E factors are based on engineering or expert judgement. The U.S. EPA has recently expanded this approach to include a letter based rating of the emissions estimate as well as for the emission factor. While there are some guidelines for the assignment of the letter score, this approach is largely subjective.

A similar method has been used in Great Britain for assessing the overall quality of emissions estimates.[21] In this approach letter ratings are assigned to both emission factors and the activity data used in the emissions estimates. The combined ratings are reduced to a single overall score following an established schedule. The emission factor criteria for the letter scores are similar to those applied in the U.S. EPA's approach and scores for the activity data are based largely on the origin of the data. Published data either by a government agency or through an industry trade association are assigned C ratings and extrapolated data based on a surrogate would receive an E rating.

The IPCC has included a rating scheme in its guidelines for reporting of greenhouse gas emissions through international conventions.[22] This scheme uses a different approach. For each pollutant associated with major source categories a code is specified to indicate the coverage of the data included in the estimate. The codes indicate if the estimate includes full coverage of all sources or partial coverage due to incomplete data or other causes. Additional codes can be specified to indicate if the estimate was not performed, included in some other category, not occurring or not applicable. An additional rating is then applied to each pollutant for each source category to indicate the quality assessment of the estimate as either high, medium, or low quality. Two additional ratings are requested that apply to the source categories without reference to specific pollutants. These ratings cover the quality of the documentation supporting the estimates, rated as either high, medium, or low; and a rating to indicate the level of aggregation represented in the estimate. The possible choices are 1 for total emissions estimated, 2 for sectoral split and 3 for a sub-sectoral split. This rating scheme has more detail but retains a simplicity that allows the analyst to quickly review the quality ratings and to compare the quality ratings to other estimates.

Another rating approach has been developed and is being used by researchers in the Netherlands.[23] This approach recognizes the difficulties in getting agreement from several organizations in international efforts on the specific needs of emissions data quality and on definitions of data acceptability criteria. In this approach two specific issues are addressed concurrently in the rating scheme. The first is an assessment of the accuracy or uncertainty in the emissions estimate, and the second is an assessment of whether decision makers have confidence in the application of the estimates for regulatory and policy activities.

In this approach two scaling indicators are applied to represent these two concerns. The first is a letter grade from A through E that indicates the inventory developers assessment of the overall quality of the estimate. A ratings imply the highest quality and accuracy and E ratings imply that the estimate is an educated guess. The second rating scale applies a letter code to indicate the purpose for which the estimate was prepared and offers the policy maker a quick assessment of the reliability of the estimate for a given application. These rating categories and their associated applicability are listed below.

Applicability Rating	Description
N	National Level
R	Regional Level
L	Local Level
I	Industry Level
P	Plant Level

This indicator is meant to provide information to the user to enable judgment of the level of aggregation put into the estimate. For example. when an emission factor is based on national averaged numbers and therefore aimed at estimating the national total emissions, it is assigned a rating of "N", and the user would be cautioned against the application of this factor for any specific plant, or for only one section of a country where conditions may be different. Likewise estimates based on plant level data, with a rating of "P", would not be used with high confidence to estimate the regional total emissions for an emission sector.

One more quantitative approach to address this need is being developed by the Office of Research and Development of the U.S. Environmental Protection Agency.[13] In this approach a numerical value is associated with the quality of the various components or attributes of an emissions inventory. This technique, called the Data Attribute Rating System (DARS), seeks to establish a list of attributes that can affect the quality or reliability of the emission factor and activity data associated with the emissions estimate for any given source category. A numerical scale is used to rank these attributes in a relative priority against a set of criteria selected to represent the reliability of each attribute estimate. This procedure will allow a comparative assessment of the overall quality of the alternate emissions estimates for a specific category or for a group of high priority source categories in an urban or regional inventory. Some additional details of this proposed approach are provided in Appendix A and further information will be available during 1995.

An Example of a Data Quality Rating Approach

Table 7 represents an application of the concepts of qualitative data rating schemes for the most important pollutants of concern in air quality analyses organized by major source category groupings. It is important to note that any such qualitative summary is subjective and that individual researchers may not agree with every entry listed in the table. While the subjective nature of this approach is recognized, the data ratings summarized in Table 7 represent a general consensus among the members of the UN/ECE Expert Panel on Verification, given the current understanding of emissions inventory estimation methods. The letter grade ratings summarized in Table 7 are primarily applicable to the estimation approaches for emissions inventory preparation that rely on emission factors and estimates of activity indicators. In all cases, the application of more direct approaches based on measurement would receive higher quality ratings.

The application of these subjective ratings for the aggregated source category groupings represented, can be misleading in some cases. For example, the rating specified for heavy metals/persistent organic pollutants for road transport is listed as E to apply in general to the understanding of the contribution of these pollutants from mobile sources. In fact for the specific case of lead from mobile sources the emission factors and emissions estimates are known with

TABLE 7. EMISSION INVENTORY UNCERTAINTY RATINGS

SOURCE CATEGORY GROUPING		SO_2	NO_x	VOC	CO	NH_3	HM/POP	CO_2	CH_4	N_2O
1 public power, cogeneration and district heating		A	B	C	B		D	A	C	E
2 commercial, institutional & residential combustion		B	C	C	C		E	B	C	E
3 industrial combustion		A	B	C	B		D	A	C	E
4 industrial processes		B	C	C	C	E	E	B	D	D
5 extraction & distribution of fossil fuels		C	C	C	C		E	D	D	
6 solvent use				B			E[1]			
7 road transport		C	C	C	C	E	E[2]	B	C	E
8 other mobile sources and machinery		C	D	D	D		E	C	D	D
9 waste treatment and disposal activities	incineration	B	B	B	C		D	B	C	E
	other	C	C	C	C	E	E	C	D	E
10 agriculture activities			D	D	D	D	E	D	D	E
11 nature		D[3]	D	D	E	E	E[3]	D	E	E

[1] In some cases, solvents may be toxic compounds

[2] Rating representative of typical pollutant source category combination; some specific cases may have higher ratings

[3] Natural sources could be contributed from volcanoes and other geothermal events

significantly more confidence. In such an analysis at that level of disaggregation, lead from mobile sources would receive a B rating. Also at this level of aggregation several source category pollutant combinations are irrelevant in that emissions of the pollutant from that source category are zero or so minimal as to be of little or no importance.

The value of a rating scheme such as that summarized in Table 7 is enhanced when applied in conjunction with a table of total emissions from each pollutant organized in the same matrix format. The researcher can then compare relative quality ratings in consideration of the overall contribution of that category to the total loadings of emissions of the specific pollutant species. The appearance of sources of significant amounts of pollutants with corresponding low quality ratings can serve to caution researchers on the applications of the inventory and direct efficient research efforts in future programs to improve the quality of the overall inventories.

SUMMARY

In summary, procedures for estimating emissions uncertainty have only recently been made available for specific, well-understood emissions sources and the pollutants that are unmistakably associated with those sources. While these techniques are useful to assess the relative accuracy and validity of the aggregate emissions estimates, they have not yet evolved to the level where they can be rigorously applied to sensitivity studies of photochemical air quality models and other more detailed analyses associated with emissions control options and control strategy development. Further efforts are ongoing and opportunities are being explored for analyses that can be used to evaluate the validity of an emissions inventory in terms of its influence on air quality analyses. Some of these opportunities will be discussed in the next section of this report.

The deficiencies in inventory development methodologies and the lack of rigorous estimates of the error in existing inventories have serious impacts on air quality analyses and air quality management programs. These concerns have been expressed concisely in a recent book published in the United States by the National Research Council:

> *The development and refinement of methods for estimating emissions is a fundamental element in the implementation of the regulatory approach to air quality management. Demonstrating the accuracy of emissions estimates has been the Achilles' heel in evaluating the effectiveness of air quality management control strategies and is a fundamental flaw in the regulatory process.*[14]

GROUND TRUTH VERIFICATION

The implementation of the procedures and activities discussed in the preceding sections of this report will provide the basis for the development of a well-documented emissions inventory database. The application of techniques to establish a likely range for the final emissions estimates, and the methodologies for the estimation of uncertainty can assist in a qualitative assessment of the representativeness and relative accuracy of the inventory data. Ground truth verification involves techniques that make direct comparisons between emissions estimates and some other known quantity that is related either directly to the emissions source or indirectly to the underlying process that results in emissions. While ground truth verification procedures can be resource intensive they will often provide the most powerful and quantitative method for data verification and should be incorporated into emissions inventory development programs whenever possible.

The purpose of this section is to discuss some of the techniques that can be applied to ground truth verification. Many of the techniques discussed in this section have been applied in the United States and elsewhere, and have provided useful insights into the major weaknesses of existing inventory estimation methodologies and resulted in additional research programs to improve these methodologies. Other promising approaches based on innovative applications of modeling and mathematical concepts are also discussed. One approach is based on the work reported by Johnson, et al,[24,25,26] that describes a unique way to analyze the urban ozone formation process. Other approaches based on artificial intelligence and the mathematical formulations associated with artificial intelligence techniques are also mentioned. The conceptual basis for these approaches is presented here, although the details of the analysis technique are necessarily limited, since practical applications of these techniques are not available.

The increase in verification studies within the global scientific community has been discussed in previous sections of this report. A valuable example of this interest is the work on verification that is being conducted in support of the IKARUS project (Instruments for Greenhouse Gas Reduction Strategies) which is discussed in a recent publication of the Research Center Julich (KFA) sponsored by the Federal Republic of Germany.[27] This research addresses many verification issues in the context of coordinated international climate change programs. One aspect of this work involves verification of emissions inventory data and other data used in support of the development of emissions inventories. This work is of particular importance to European emissions inventory development projects, because it addresses specifically the needs related to transparency of emissions and other analysis efforts that involve more than one country. This report discusses many of the specific ground truth analyses that are discussed in the remainder of this section of this report. Interested readers are encouraged to explore the IKARUS project and to consider the adoption of interesting results that will be developed through this program.

This discussion of ground truth verification techniques is organized into the three major groupings listed below. In some cases, the actual implementation of specific activities might involve elements from more than one of these groups. Some results of actual field measurement programs based on some of these techniques are discussed, for applications where such results are available. As mentioned earlier in this report, innovative mathematical approaches such as artificial intelligence, fuzzy logic, chaos theory and fractal geometry should be explored for application in emissions verification programs. Since these approaches have not yet been adapted to this application, no examples are available and they have not been discussed in this section of the report. The major groupings included here are:

- statistical survey analyses
- monitoring analyses
- modeling analyses

STATISTICAL SURVEY ANALYSES

Some common methodologies for estimating emissions from area source emission categories rely on a per- capita, per-employee, per-land area or some other surrogate emission factor. While these approaches may be adequate for estimating national or regional emissions. they may introduce bias when applied to specific locations or during specific time periods. One method for verification of emissions estimates based on a surrogate or aggregate emission factor is to perform a survey on a selected sample of the target population of individual sources included in the aggregate source category. Ferreirro and Cristobal have discussed several approaches that can be followed to select an appropriate sample for survey analyses.[17]

Although the focus of this work is related to the verification of an existing emission inventory, the approaches discussed could also be used in the development of emission factors or other parameters used in calculating emissions for a source category (activity measures, control efficiency, etc.). The discussion stresses the need to characterize the target and sampling populations and to specify the sample design as an initial step. Characterization of the source populations includes descriptions of the sectoral, spatial and temporal dimensions of the inventory; an extremely important consideration when the emission inventories developed by a number of organizations are expected to be compared, each with differing categorical schemes.
Haphazard, judgement, and probability principles are discussed as sample selection alternatives. The haphazard method is only appropriate when the target population is homogenous. Selection

of the most easily accessible sources is favored using this technique, which may introduce biases and is not amenable to assessing the accuracy of the estimates derived. The judgement method relies solely on the subjective knowledge of experts to select representative sample units. Although the use of experts is a prerequisite for developing a sound sampling design, it is difficult to verify if it is used as the sole method for choosing samples. Probability sampling includes simple random sampling, stratified random sampling, two-staged cluster, systematic, and double sampling. The first two methods are discussed in detail by Ferreirro and Cristobal. Simple random sampling assigns an equal chance of any one unit in a population being chosen. The simple random sampling method is a valid technique only if there is low variability among subsets within the target population.

Stratified random sampling benefits from simplicity of design and that reduction in the overall variance of the sampling errors can be achieved in an efficient and cost effective manner. The stratified random sampling approach is recommended whenever possible. The target population is first divided into a number of subsets which are non-overlapping and together cover the whole population. These subsets or strata should be homogenous within themselves and show diversity between themselves. Strata can be partitioned based on size, technologies, or any other attributes of the population units.

Data collected prior to a verification (i.e., in the original emission inventory) can also be used in the verification process. This is true for both the simple random sampling approach or in stratified random sampling. Care must be taken, however, to place previously collected data into the proper strata for stratified random sampling, and to assure that the samples are randomly selected before using previously collected data (i.e., sample selection should be performed before determining what data are available).

Methods for presenting the results of these analyses are also discussed, with the recommendation of the use of the box plot and K-number representations. These representations of the data depend on the median and other categorical factors to determine the sample distribution. Determination of the confidence limits is possible for these categorical factors by using either normal distribution statistics or non-parametric procedures. Another alternative is to perform a logarithmic transformation of the data to approximate a symmetrical distribution and thereby "normalize" the data before using in standard statistical techniques. Methods for testing the data for conformity to a standard distribution, identification of outliers, and testing the general consistency of the empirical data are also discussed.

An example of such an approach is the application of a per capita emission factor for estimating VOC emissions from dry cleaning operations. On average in a particular country, a per capita emission factor can provide an accurate estimate of annual emissions on the national scale. It is likely, however, that highly populated urban areas with a large concentration of service-related or government employment would have higher per-capita emissions than rural, agricultural areas. The development of total emissions using the per-capita emission factor and the distribution of those emissions based on the population spatial surrogate factors might result in a skewed distribution of the emissions rate in specific areas. It is also possible that the use of dry cleaning services could be related to seasonal factors that could affect the temporal distribution of emissions.

Statistical sampling techniques, such as those discussed by Ferrierro and Cristobal[17], could be implemented to identify the population of dry cleaning establishments that need to be sampled in detail to provide a statistically rigorous definition of the regional and temporal distribution of the activity associated with the dry cleaning industry. The results of a statistical sampling based on these principles could be applied to develop emission or allocation factors that depend on population density, economic demographics, or the distribution of employment by major industrial and commercial sectors.

These approaches may be used to develop more relevant emissions estimation methodologies or to assess the potential regional or temporal bias introduced by application of the simple population-based approach. These approaches could be applied to other source categories in addition to the dry cleaning industry. Some of these categories include autobody repair, residential wood-fuel use, and heavy-construction equipment. The application of these techniques requires an understanding of the emission sector under consideration to ensure that a representative and random sample of facilities is included in the survey.

Another possible survey approach could be implemented to evaluate the representativeness of resolved emissions estimates applied in urban modeling analyses. In this approach, some of the grid cells that are thought to contribute significant emissions magnitudes could be surveyed in a methodical way. This would involve a detailed manual survey of all stationary activities in a given grid cell location that can result in emissions. Emissions estimates for the collection of facilities in the grid cell would be developed based on material balance or other sound engineering assessment. Details of the specific chemicals used in these industries, the diurnal nature of the processes resulting in emissions, and other factors related to the emission sources could be obtained through this survey. The results of these compilations could then be compared to the emissions magnitude and temporal and species assumptions applied in the allocation approach used to develop the modeling inventory, to assess the weaknesses of those assumptions.

In survey applications, the initial sampling and manual survey could be accomplished simply to identify the facilities to be included in a follow-up survey, using questionnaires that could be sent to the facilities to acquire the required data. The use of a follow-up questionnaire would reduce the personnel resources required for the study, but would also result in a burden to those facilities selected for the survey. The use of questionnaires is also affected by the willingness of the selected facilities to respond and by any bias in the estimates of the activities associated with those facilities that would be introduced by the person or group of people who would be responsible for completing the questionnaire.

MONITORING ANALYSES

Monitoring analyses include three principal types of measurement activities: direct source testing, indirect source testing, and ambient measurements. All monitoring programs are expensive to implement and should be well planned and executed to maximize the data recovery and to ensure the collection of high-quality measurement data. It is possible, in some cases, to apply measurement data that are routinely collected as part of a government-sponsored air quality management program, and data that are routinely collected by individual facilities to monitor process operation and efficiency to an emissions verification exercise. Whenever a monitoring program is considered, a thorough review of all existing measurement data should be completed and the program should be designed to make use of these data whenever possible. Table 8 presents a summary of the potential uses of monitoring data for emissions inventory verification.

Direct Source Testing

Direct measurement of stack gas emissions, using CEMs, is sometimes required to establish compliance with environmental regulations. Obviously, if such measurements are available to the agency responsible for the development of an emissions inventory, those data can be applied directly to the inventory. In these cases, there is no need for the application of an emissions estimation technique. More commonly, however, such compliance data are only available for limited periods of time, or for only a subset of the population of sources in a given area. However, compliance data collected for some specific facilities or over a limited time period, along with similar data collected specifically for application to an emissions verification program, can be used to evaluate emission factors and emissions estimation techniques.

The application of this type of direct source testing data simply involves the comparison of the emission factor derived from the measured data to the emission factor used in the estimation technique or the measured emissions to the emissions calculated through the application of the estimation technique. When using compliance data, it is important to consider the operating conditions in effect during the test. In many applications, compliance tests are performed during periods of maximum load. If normal operating conditions are at a slightly reduced load, the results of the compliance test under maximum load may result in a bias when compared to the estimation technique.

TABLE 8. MONITORING TYPES, EXAMPLES, AND USES FOR EMISSIONS INVENTORIES

Monitoring Class	Examples of Monitoring Programs	Uses of the Data for Emissions Inventories
Direct Measurements	• Inprocess emissions measurements • Process operating parameters • Random sampling of process units or potential leak tests	• Comparison to estimated values • Identification of ranges of application estimates (operating parameters, emissions factors) • Specification of fugitive emissions or process leaks
Indirect Measurements	• Remote measurement systems: FTIR, UV, Gas Filter Correlation • Ambient VOC/NO_x ratio studies	• Comparison of estimated emission rates with near source concentrations • Estimation of emission factors for sources that do not have stacks or vents
Ambient Studies	• Tunnel Studies • Aircraft Studies • Upwind-downwind difference studies • Receptor Modeling	• Identification of obvious weaknesses in procedures or underestimation of emissions • Checking of ambient impacts of sources or mixtures of sources • Identification of principal emissions sources in a region

The U.S. EPA and Environmental Agencies in other industrialized countries have published a series of standard methods for application to emissions testing of stationary sources. These standard methods have been developed to promote consistency and comparability between independent measurement programs.

The U.S. EPA has also established methods for testing highway gasoline-powered motor vehicles. Many States and local agencies have adopted the Federal motor vehicle test procedures or variations of those procedures, known as motor vehicle inspection and maintenance (I/M) programs, as part of their air quality management plans. Although the I/M programs are designed to identify in-use vehicles that do not comply with Federal emissions standards, they are in fact a direct source emissions test. Applications of these tests and the experience gained through their routine operation in many urban areas in the United States has led to the development of assumptions about the distribution of emission rates in the overall vehicle fleet. These tests monitor directly the exhaust gas generated during idle and/or specific load conditions.

Indirect Source Testing

Direct source testing methods are primarily applied to large stationary sources where emissions are vented through a clearly identifiable stack or vent. Indirect source testing methods are used to estimate emissions from dispersed sources. These types of sources are either too numerous to consider individually , like residential space heating, or arise from unexpected sources, like leaks in chemical plants or petroleum refineries. Some examples of indirect source testing are described below.

Measurement of Operating Parameters. It is not always necessary to measure the direct emissions from a source to quantify the actual emissions. For sources that have relatively high-quality emission factors or emission estimation algorithms that have been demonstrated to predict emissions with a high degree of accuracy over the typical range of operating conditions, emissions can be monitored by collecting and processing these operating rate data. For example, SO_2 emission factors for coal- and oil-fired boilers are relatively well known. These emission factors are expressed as a function of the sulfur content of the fuel. Therefore, accurate monitoring of the fuel use rate and the sulfur content of that fuel can be applied to make highly accurate estimates of the SO_2 emission rate as a function of time.

Random Sampling of Leak Sites. Developing emissions estimates for fugitive losses of VOCs from equipment and process leaks in large, complex chemical plants, pharmaceutical manufacturing facilities, and petrochemical refineries is particularly difficult. Typically, emission factors based on an average measured emission rate for pumps, flanges, valves, storage equipment and process equipment, are applied to all similar plants, even though emissions measurements for those specific plants are not available. Any generic approach based on this general methodology will introduce bias when applied to specific operating facilities. Differences in operating conditions, chemicals used, maintenance procedures, and products produced in individual facilities contribute to the potential for bias when applying these techniques. In addition, the emission rate measurements frequently focus on those devices that are characterized as being the most significant leaking sources. One more refined approach is to routinely monitor a random sample of these emission points in an individual facility to apply a statistically representative distribution of those data to all of the potential leak sites. In this approach a more representative emission estimate can be developed for any individual facility without the need for direct measurement of all of the specific leak sites in operation at the facility.

Remote Measurement Techniques. The sampling procedures used in direct emissions source tests are based primarily on the collection of a captive sample, which is then directed to an analysis cell or enclosed in an airtight container that is delivered to a controlled laboratory setting for analysis. These types of measurements are frequently referred to as in-situ sampling techniques. Remote measurement techniques are measurement methods that do not rely on the collection of the captive sample. Instead they make a determination of concentration or some other physical property in an undisturbed air parcel. A common remote measurement method that is familiar to everyone is radio detection and ranging, or radar. Radar systems can pinpoint the location of a mass that reflects radio waves emitted from a centrally located transmitter. The vector and time delay of the radio reflection identify the location of the mass that is measured. Similar principles can be applied to measure the concentration of gases in air. Some examples of remote measurement technologies applicable to measure air quality parameters include the following:

- light detection and ranging (LIDAR)
- differential absorption LIDAR (DIAL LIDAR)
- Fourier transform infrared spectroscopy (FTIR)
- ultraviolet (UV) spectroscopy
- gas-filter radiometer

Each of these technologies can be used to measure the concentration of pollutants along a line of sight through the ambient atmosphere or at the mouth of an emissions source. The measurement principle of all of these techniques is based on the physical properties of molecules that serve to alter the wavelength or intensity of light waves as those light waves pass through an air sample. All molecules have properties that result in the absorption of characteristic wavelengths of electromagnetic energy. The energy that is absorbed by the molecules alters either the vibrational, rotational, or electron orbit energy state of the molecule. Simply stated, the measurement is performed by monitoring the change in the energy signal of the light between the light source and the light receiving equipment. The LIDAR techniques involve a narrow waveband laser as a light source. The infrared, ultraviolet, and gas-filter correlation spectroscopy techniques use a lower power light source that emits energy over a wide range of wavelengths.

All of these measurement techniques are experimental and only FTIR and Gas Filter Radiometry have been used in field tests to explore opportunities in emissions measurements programs. These techniques may have applications in emissions verification programs in the future. The following sections present a brief summary of some of the experimental applications of these technologies.

Example of an FTIR Emissions Test. The U.S. EPA Office of Research and Development is supporting research to demonstrate the application of remote measurement systems based on FTIR technology for estimating emission rates from large dispersed area sources.[28]

These particular tests were performed to evaluate the technique in measuring emissions from a surface coal mine to develop an emission factor. However, the method could just as easily be applied to check or verify the results of an emission estimation methodology for the source. The example discussed here is designed to measure methane (CH_4) emissions from surface coal mining operations, but the basic approach could be applied to other similar sources including but not limited to; landfills, waste water treatment systems, emissions from agricultural pesticide application, controlled field burning, and wildfires. Adaptations to the basic approach are also being explored by U.S. EPA to measure emission rates from other industrial activities such as fugitive emissions from process leaks, and fugitive emissions from chemical storage facilities.[29]

The approach involves the measurement of a path averaged concentration along a line of sight that is immediately downwind of the area source. In the application described here, the line of sight measurement was obtained at approximately one meter above the surface along the lip edge on the downwind side of the coal pit. The application of the method requires simultaneous measurements of the wind speed and direction, temperature, and atmospheric pressure. These parameters are used to estimate the shape and extent of the emissions plume using simple dispersion modeling techniques. The path average measurements are used along with the results of the simple dispersion modeling techniques to calculate the emissions source strength required to produce the calculated plume.

The results of these tests provided reasonable emissions estimates; however, experimental and equipment problems were encountered during the exercise. Following these preliminary tests, EPA initiated additional research to evaluate the technique and to further develop the approach. These tests were carried out in a research field in the Research Triangle Park area of North Carolina in the summer of 1992.

The results of the tests were encouraging. A large percentage of the experiments yielded calculated emission rates within 25 percent of the known emission rate from a simulated area source. Meteorological factors do affect the results of the modeling approach. Research efforts to refine these methodologies for use in emissions factor development and leak detection from volume sources are currently being supported by the U.S. EPA Office of Air Quality Planning and Standards.[29]

Another application of FTIR measurements of emissions from wildfires in Australia has been reported.[30] In these experiments, emissions of CO_2, CO, CH_4, CH_2O, CH_3OH, HCOOH, CH_3COOH, NO, NO_2, NH_3, N_2O, and HCN were obtained simultaneously for several grass fires and fires of piled forest debris. The emissions of all compounds were expressed as a ratio relative to the emissions of CO_2. The tests conducted in these experiments provide good examples of the use of the FTIR open path measurements as an emissions verification technique. The results of the study indicate higher than expected emission rates for reduced and partially reduced species including NH_3, CH_4, and CH_2O. In fact, the results of these tests revealed that NH_3 was the dominant form of nitrogen emissions from these fires. Conventional thought would not have predicted that the emissions of NH_3 would be higher than the oxidized forms of nitrogen.

Example of a Gas-Filter Radiometer Emission Test. Researchers at the University of Denver have developed a gas-filter radiometer that is used to remotely measure emissions of CO from in-use highway motor vehicles.[31,32] The system uses an infrared light source that is mounted on one side of a single lane road segment. In these tests measurements were made on an on-ramp to a restricted access highway. The detector unit is operated on the other side of the roadway. The line of sight is set at approximately 10 inches above the road surface to be in line with the exhaust pipe. The instrument uses three detectors, one for CO, one for CO_2, and one as a reference channel. As each car passes the detector, there is a drop in the reference signal caused by the car interfering with the light beam. This drop in the reference initiates a measurement. As the car exits the beam, a one-second voltage versus time trace is obtained and stored electronically in the device. The system uses a rotating filter wheel, with one cell filled with CO and H_2 and the other cell filled with N_2.

A freeze-frame video system is used to make a permanent record of each vehicle tested. This system can be operated unattended and more than 1,000 vehicles can be tested per day. After the test period, the system is retrieved and taken to the laboratory where information is downloaded into computer-based files for further processing. This instrument has been operated through several measurement periods and has collected CO emissions data for more than 117,000 individual cars. An instrument based on a similar method but without the gas-filter wheel has been developed by General Motors Corporation.[33] Both of these instruments have been operated in side-by-side tests to verify that they give comparable results.

These systems are primary examples of the use of indirect source measurements for inventory verification. The results of the measurements were compared to emissions estimates obtained by use of the standard MOBILE4 motor vehicle emission factor model and the EMFAC7 motor vehicle emission factor model developed by the State of California. In all such tests, a significant discrepancy was found between the CO emissions estimates predicted with the models and the resulting CO emission rates measured with the instruments. The results of these studies indicate that 50 percent of the CO emissions from all vehicles result from less than 10 percent of the cars. The standard motor vehicle emissions models do not adequately treat the high emitting vehicles and, consequently, underestimate total exhaust emissions. These indirect measurement methods of in-use vehicles are more representative of actual fleet emissions than controlled tests in I/M programs because vehicle owners can plan for and make adjustments to the onboard emissions control equipment prior to the I/M tests, yielding tests that are not representative of the actual conditions under which the vehicles are operated in normal use. In-use measurement studies have identified the use of the standard motor vehicle emission factor models as a major source of error in urban VOC and CO emissions inventories. The results of these studies provide excellent examples of measurements-based approaches to emissions inventory verification projects that can help focus future research and method development that will result in improvements in emission inventory estimates.

Ambient Measurements

Several techniques have been developed and applied that seek to relate ambient measurement data to emissions source strengths. The studies using these techniques have been conducted to assess the reliability of general overall emissions estimation methods for use in regulatory applications. These studies can be categorized in one of three major groupings: ambient ratio studies (VOC/NO_x and CO/NO_x), tunnel studies, and receptor modeling studies. The concepts of using these types of studies for emissions verification and some examples of each are discussed in the following paragraphs.

Ambient Ratio Studies. In the United States, ambient measurement programs are routinely operated in urban areas that are classified as nonattainment for the ambient ozone standard. Typically, these measurement programs include a rural measurement site in a location that is in the typical upwind sector, two or more sites in the downtown area near the urban core, and two or more sites in the downwind sector at locations that are thought to represent the location of the ozone maxima events. Both grid-based and trajectory modeling approaches are used to simulate the urban area and model predictions are compared to the observed concentrations of ozone and ozone precursors. The use of grid-based models allows the investigator to track the temporal distribution of ozone precursors in the urban center in addition to the ozone maxima. Frequently, these models are reasonably successful in predicting the ozone maximum in the downwind locations, but are less successful in tracking the concentrations of precursors in the downtown area. These types of results have led researchers to question whether the underlying emissions inventories are adequately representing the actual emissions fields, and to question if control strategies based on these modeling predictions are valid.

A detailed research study, sponsored by the California Air Resources Board (ARB), has been completed to assess the ability of standard emissions inventory estimation methodologies to adequately represent the concentrations of nonmethane organic gases (NMOC), CO, and NO_x, and the ratios of $NMOC/NO_x$, and CO/NO_x observed in selected regions of the South Coast Air Basin surrounding Los Angeles.[8] In this study, ambient air measurement data were evaluated to estimate the $NMOC/NO_x$ and CO/NO_x under various temporal scenarios in regions that are primarily influenced by highway motor vehicle emissions. Similar ratios were determined from the gridded, hourly, and speciated emissions inventory under a variety of spatial averaging assumptions.

Statistical analyses were performed to determine the most appropriate temporal scales for these comparisons. Ratios derived from early morning measurements (7 to 8 a.m. local time) were the most appropriate for comparisons of the NMOC/NO_x and CO/NO_x in the summer months, and similar ratios derived from overnight measurements were found to be most appropriate in the fall months. Spatial averaging was evaluated for the single grid cell covering the measurement site, for multiple grid cells surrounding the measurement site, and for the basin average emissions estimate. In the summer months, comparisons between the measured data and the highway motor vehicle inventory were analyzed, and in the fall months some contribution of stationary source NO_x emissions was included. The results of the study suggest that the measurements-based ratios for NMOC/NO_x and CO/NO_x are about 2 to 2.5 and 1.5 times higher, respectively, than the corresponding ratios derived from the emissions inventory. If it is assumed that the NO_x emissions inventory is representative of the motor vehicle NO_x emissions, these results suggest that current mobile source emissions methodologies underestimate NMOC and CO emissions by those factors. Other measurements-based ambient data collected from tunnel studies (discussed below) suggest that the overall NO_x emissions from motor vehicle sources is reasonably estimated from existing emissions methodologies. Further modeling exercises using grid-based photochemical models yield similar discrepancies between the measured and estimated emission rates.

Additional studies, designed to evaluate the comparisons of ambient NMOC/NO_x ratios with those derived from emissions inventories, have been conducted by the U.S. EPA. In the first study, similar comparisons of NMOC/NO_x ratios derived from ambient measurements and emissions inventory estimates were developed for 15 cities in the United States.[9] The emissions inventory ratios were based on county wide emissions estimates taken from the 1985 NAPAP emissions inventory database. The baseline comparisons in this study showed that, on average, the emissions inventory ratios were 24 percent lower than the ratios derived from the ambient measurements. The baseline emissions inventory was modified to include enhancements to account for biogenic VOC emissions, to update the mobile source emissions to be representative of MOBILE4, and to account for rule effectiveness assumptions. The comparisons based on the modified inventory data were, on average, 2 percent lower than ratios based on the ambient measurement data. Comparisons for individual cities ranged from a value where the inventory-derived NMOC/NO_x ratio was 173 percent higher than the measurements-based ratio to a value where the inventory ratio was 61 percent lower than the measurement ratio.

Further analyses on four cities including (Houston, Texas; Philadelphia, Pennsylvania (two sites); St. Louis, Missouri; and Washington, DC) were explored in a follow up study.[10] In these analyses, gridded emissions data based on the NAPAP inventory were compared to measurements-derived ratios for measurement sites contained within the grid cell. The same enhancements were made to the emissions inventory data, although in these tests the effect of the biogenic component was minimal since the comparisons were made during early morning hours and the sites were urban areas with little vegetative cover.

The results of these studies suggest that on average the NMOC concentrations derived from the inventory data were underestimated by 50 to 80 percent relative to the ambient measurements. At one site, the emissions inventory overestimated NMOC concentrations by about 20 percent. The emissions inventory data for Houston, however, underestimated NMOC concentrations by 330 percent. This result may include bias due to the neglect of potentially significant point source NMOC emissions resulting from the large population of petrochemical industry sources in that area, which are outside of the selected grid cell. With the exception of the data for Houston, the discrepancy between emissions derived NMOC and ambient NMOC was not strongly dependent on ambient temperature, implying that the sources that are underestimated in the emissions inventory are not temperature- dependent. The Houston data did show a significant relationship to temperature, suggesting that sources such as organic liquid storage may be the cause of the emissions that are not adequately reflected in the inventory.

There are several other examples of similar or related studies to assess the relationships between emissions inventory-derived NMOC/NO_x and CO/NO_x ratios and those derived from ambient measurements. In all cases, the trend is toward underestimation of VOC emissions in the emissions inventories. Each of these studies is based on simplifying assumptions that can affect the comparisons and, therefore, should be viewed as preliminary. The consistent results indicating moderate to significant underestimation of VOC emissions, however, leads to the conclusion that most emissions inventories underestimate VOC and CO emissions in the aggregate, and the development of emissions control strategies based on these inventories may be inadequate to achieve the desired reduction in ambient ozone and CO concentrations.

The U.S. EPA Office of Mobile Sources recently completed a study to review 5 specific studies of comparisons between ambient VOC/NO_x and CO/NO_x ratios and similar ratios derived from emissions inventories.[34] This study concludes that these ratios in ambient monitoring data are higher than those calculated from emissions inventory data, suggesting that the VOC and CO inventories underestimate actual emissions or that the NO_x inventories overestimate actual emissions. There are several problems related to source distributions and mixing assumptions that influence these results. Additional efforts are required to establish the true meaning of these types of comparisons, but the studies completed so far have provided useful first steps to a potentially valuable emissions verification tool.

Tunnel Studies. Highway tunnels offer an excellent location to sample the contribution of emissions from in-use highway vehicles. Tunnel studies were first used in the United States to estimate in-use emissions rates from highway vehicles in 1981.[35] More recently, a study was completed in 1987 in a tunnel under the Van Nuys airport runways in the Los Angeles area.[36] In the Van Nuys study, concentrations of VOC, CO, NO_x, and particulate matter (PM) were measured at both the upwind and downwind portals of the tunnel and the emissions rate was measured by difference. Air flow was determined by simultaneously monitoring the exit concentration of an SF_6 tracer, which was introduced at the upwind portal at a known release rate. Video images were recorded to accurately assess the distribution of vehicles in the tunnel during the measurement periods. Average vehicle speed was measured in each lane of the tunnel during each experiment. Altogether 22 measurement periods were monitored during October and December of 1987. The measured concentration data were used to estimate the mass emissions rate for the sampling periods.

The temperature, vehicle type distribution, and average vehicle speed data were applied in the California mobile source emission factor model (EMFAC7) to calculate the mass emissions rate for each monitoring period. The emissions rates estimated from the EMFAC7 model were then compared with those derived from the measurements. In all 22 measurement periods, the emissions rates of VOC and CO, based on the measured concentration data, exceeded those predicted by the emissions model by factors of 1.4 to 6.9, and from 1.1 to 3.6 for VOC and CO, respectively. The comparisons for NO_x, however, were very consistent with those predicted by the model. Ratios of measured to modeled emission rates for NO_x varied from 0.6 to 1.4, with a mean ratio of 1.0. These results suggest that the EMFAC7 model is adequate for estimating NO_x emission factors but consistently underestimates emission factors for both VOC and CO. If only VOC emissions were underestimated it might be concluded that the EMFAC7 model did not adequately treat running loss evaporative emissions. Since both CO and VOC are consistently underestimated, however, it is more likely that the EMFAC7 model fails to account for the percentage of vehicles that are gross emitters. It is assumed that the vehicles using the tunnel over this time period represent a random sample of the overall vehicle fleet in the Los Angeles area. The use of EMFAC7, therefore, could underestimate basin-wide motor vehicle emissions by a factor of 2 to 5. The consistent underestimation of VOC and CO emissions from motor vehicle sources has serious implications on the development of area-wide control strategies based on emissions inventories that are developed through the use of the EMFAC7 or MOBILE4 mobile source emission factor models.

The earlier studies completed in the Allegheny Tunnel[35] also imply a consistent underprediction of emissions by mobile source emission factor models. The earlier studies suggest a consistent underprediction of VOC, CO, and NO_x by the models. It is difficult to compare the studies, however, because earlier studies used earlier versions of the mobile source emission factor models that have since been updated to include additional evaporative loss emissions. Comparisons between the results of these two tunnel studies are further complicated by differences in the mix of vehicle model years, the mix of vehicle types, and the speeds associated with traffic in the two tunnels.

Aircraft Monitoring Studies. Results from an interesting measurement program have been reported by researchers at the TNO Institute of Environmental Sciences.[37] This paper presents results of study comparing emissions inventory results to ambient monitoring results using an instrumented aircraft platform. Aircraft measurements are made in both the upwind and downwind direction from a cluster of sources of specific VOC emissions. The measurements are obtained at various altitudes to define a flux of the selected pollutants in both locations and the difference is attributed to the combined emissions strength of all sources in the area within the measurement planes. In these preliminary studies the analyses focused on the major known sources of a list of five specific VOC species representative of the source mix being studied. The results of the study indicated a significant potential of this methodology to verify emissions inventory procedures. Although the estimates of the emission strengths determined from the aircraft measurements were consistently higher than the source strength estimated from the inventory, the ranges of emissions estimates determined by the two estimation approaches overlap in general. These results are encouraging and indicate that further exploration of this and other related techniques should be explored in future studies.

Receptor Modeling. Receptor modeling is the use of ambient measurement data and the chemical characteristics of specific source types to estimate the contribution of different sources to the observed concentration of pollutants in a sample. The most common use of receptor modeling techniques is in chemical mass balance (CMB) receptor modeling analyses. CMB studies rely on the known distribution of VOC species in the major sources or source categories in an area. The specific compounds selected for analyses are known as the fitting species. The criteria for the selection of fitting species is that they cannot be emitted in large amounts from other sources, and they cannot be subject to photochemical reaction during transport between the emission point and the receptor monitoring location. For instance, acetylene is a primary component of motor vehicle exhaust and is not emitted in large quantities from other types of sources. Acetylene is also relatively unreactive in photochemical systems and, therefore, the acetylene concentration measured in an ambient air sample can be assumed to result from motor vehicle exhaust. The concentration of the fitting species in a given air sample relative to the total VOC concentrations can be used to estimate the relative contribution of that source to the measured VOC concentration. In this way, the relative contribution of the major sources can be assessed.

In one example, the U.S. EPA has performed a CMB receptor modeling analysis of ambient air samples collected in Atlanta, Georgia, during the summer of 1990.[38] This study was a preliminary analysis to demonstrate the technique and only the contribution of mobile sources was estimated. The Atlanta area is a good location for use of this analysis technique to estimate the contribution of mobile sources because high-quality mobile source speciation data were available and mobile sources dominate the VOC emissions in the Atlanta area. The results of the study suggest that 77 percent of the VOC emissions result from mobile sources. Other studies that provide the split between mobile sources and stationary sources have also been suggested for the Atlanta study area. Similar studies can be implemented in any urban area that has a relatively complete measurement program that provides speciated VOC measurement data. These studies can be used to determine whether the emissions inventory database adequately represents the relative contributions of general source categories. Receptor modeling approaches can also be used to estimate the relative contributions of individual facilities in a group of four or five adjacent industrial facilities. In this application of receptor modeling, ambient concentration excursions over small time scales are analyzed relative to short-term variations in winds in the immediate study area. These data can be interpreted with dispersion models to locate the specific source regions of the fitting species. These analyses can be used to construct the distribution of emissions magnitudes for the individual sources in the group of industrial facilities.

An approach for a more complex application of receptor modeling analyses has recently been presented.[39] In this approach, functions that describe the transformation of pollutants due to photochemical reactions can be applied to account for the mix of sources that contribute to the observed ozone precursors. The model proposed for these analyses is a hybrid receptor model, called the source identification through empirical orthogonal functions (SITEOF). The model relates gradients of empirical orthogonal functions and winds to the sum of sources and sinks of a pollutant. The model was applied in a test case, and provided qualitatively reasonable estimates of the formation rates for ozone in both winter and summer. These results could be applied along with trajectory analyses to analyze the distribution of emissions represented in the emissions inventory to those contributing to the formation of ozone derived through the receptor modeling approach. The details of application of these techniques are complex and further reading is suggested to any interested reader.[39,40]

A receptor modeling approach based on filter samples and combined x-ray fluorescence (XRF) and instrumental neutron activation analysis (INAA) has been applied to identify the sources of particulate matter collected in ambient urban environments.[40] The technique uses the chemical mass balance approach and has been used to estimate the relative contribution of various sources to the ambient particulate concentrations in Philadelphia, Pennsylvania. The results of these studies indicate that the vehicle exhaust portion of the PM-10 measurement was between 4 and 6 percent, stationary sources contributed 5 percent, and the sulfate component of PM-10 was between 49 and 54 percent. Model trajectory analyses indicated that approximately 80 percent of the sulfate particulate resulted from local sources. Further applications of these techniques have been combined with computer-controlled scanning electron microscopy (CCSEM) and transition electron microscopy (TEM) to enhance the data collection and resolution capabilities of these techniques.[41] The combined use of the electron microscope data, which provides particle morphology information in addition to the chemical composition information obtained through XRF and INAA, allows greater resolution of the source characteristics and enhances the resolution at which source contributions to the ambient particle loaded can be determined.

Integrated Empirical Rate Model. A unique methodology appropriate for the study of urban ozone formation processes has been developed by Johnson, et al, in Australia.[24] The approach, known as the integrated empirical rate (IER) model, simplifies the representation of ozone formation processes relative to the gridded, emissions-based modeling approaches that have been common in the United States and elsewhere for the past 15 years. The IER model was developed to simulate a series of smog chamber experiments that were performed under conditions that are actually observed in Sydney, Australia. Sydney is a large city with a mix of mobile and stationary sources of ozone precursors that is representative of most industrial urban areas. Smog chamber experiments performed in the United States are operated under conditions of VOC and NO_x concentrations and VOC/NO_x ratios that are atypical of actual urban conditions. This is because, in the United States, ambient air is used to flush the chambers, and it is necessary to charge the chambers with elevated concentrations of the ozone precursors to overcome the effects of precursor concentrations in the ambient air. In the Australian experiments, a high-efficiency clean air generator was employed, which allowed the researchers to obtain a highly purified background condition. The ability to establish a clean background allows simulations of VOC and NO_x conditions that represent ambient urban conditions.

The basis of the IER approach relies on the representation of the ozone formation process on a temporal scale as a function of cumulative sunlight rather than as a function of time of day. In more traditional analyses, the ozone concentration is plotted, whereas in the IER approach the net photochemical oxidation is plotted. The net photochemical oxidation is defined as the sum of NO to NO_2 transformations plus the ozone production. Figures 3 and 4 represent actual smog chamber data collected by the Australian researchers, as a function of time of day and as a function of cumulative sunlight, respectively.

The striking observation of these plots is that, in the IER representation (Figure 4), oxidant formation is a linear process as a function of cumulative sunlight, with a maximum that is defined by the initial amount of NO_x available in the system. Johnson labelled the portion of the ozone formation process characterized by the linear increase the light-limited regime, and the maximum possible ozone formation the NO_x-limited regime. The slope of the line in the light-limited regime is then a direct measure of the hydrocarbon reactivity of the sample. A less obvious but more important observation of these plots is that the inherent reactivity of the hydrocarbon mix available

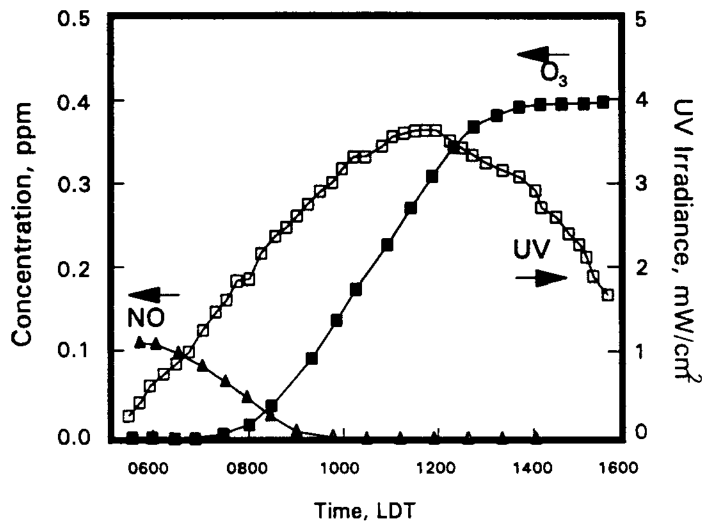

Figure 3. Ozone Formation as a Function of Time of Day

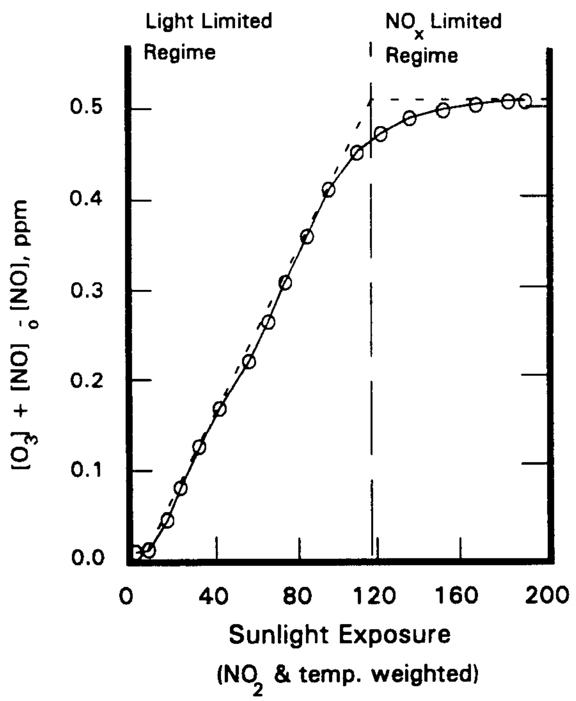

Figure 4. Oxidation as a Function of Cumulative Sunlight Intensity

in the system is conserved with time during the light-limited regime. Ambient measurements of ozone, NO, NO_2, and VOC can be analyzed to locate the air sample on the line representing the light-limited regime. It is then a simple process to translate the cumulative sunlight intensity into elapsed time, and to estimate the origin of the emissions sources by performing a back trajectory analysis.

This approach can provide a significant opportunity for emissions verification to assess the usefulness of emissions inventories prepared for the modeling-based regulatory applications. One application of the approach would use the assessment of reactivity and oxidant formation on an iterative basis to account for the contribution of emissions sources in each grid cell during each hour. The results of these analyses would provide a high-resolution estimate of the total emissions of reactive VOC and NO_x. Comparisons of these estimates to those developed through the standard inventory preparation and allocation methodologies would identify those critical regions that contain sources that are inadequately treated by current inventory methodologies. The results of the analyses could be used to identify those particular source types that have the greatest impact on ozone formation processes and ultimately on ozone control strategies.

A Measurement Instrument Based on IER. One result of the research conducted by Johnson, et al, is the development of an air quality measurement instrument that is designed specifically to measure the chemical properties associated with the IER.[42] The system This automated measurement system, called AIRTRAK monitors the NO, NO_x, ozone, photochemical oxidation, and reactivity of samples. The system can be automated to collect canister samples for laboratory analysis of speciated hydrocarbons. The advantage of this device is that it can be programmed to collect the canister samples during regularly scheduled periods, such as 6 a.m. to 9 a.m.; during periods when a significant reactivity event is occurring; or when there is a change in the oxidant formation rate. This would concentrate measurement resources on significant events rather than on collecting routine measurements, many of which are of limited interest. The use of a network of AIRTRAK instruments would provide base information that could be applied to the model-based inventory verification approach discussed above, in addition to providing all of the information routinely collected in standard monitoring programs.

The Lake Michigan Ozone Study used four AIRTRAK measurement systems during the summer 1991 sampling period.[43] The data were transferred to Australia for analysis by the instrument developer. Results of these and additional measurement applications of AIRTRAK are expected soon, to establish the capabilities of the instrument for air quality and emissions estimation applications.

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APPENDIX A

SUMMARY OF THE PROPOSED DATA ATTRIBUTES RATING SYSTEM

One of the recommendations of this report is to complete statistical uncertainty analyses or direct source measurements for specific components of any emissions inventory whenever it is possible. These forms of verification are superior to all others because they provide a quantitative assessment of the accuracy and reliability of the emissions inventory estimates.

Since direct measurement programs are prohibitively expensive in almost all inventory development programs and the data required to perform statistical uncertainty analyses are often unavailable, it is desirable to have an alternate approach that will provide some measure of a semi-quantitative assessment of the quality of emissions inventory data. The report suggests that as a minimum some form of data quality rating approach be implemented. These data quality rating schemes are subjective and at best offer a qualitative assessment of the overall accuracy and reliability of the emissions estimates. One option to provide a more quantitative quality rating method is being developed by the Office of Research and Development of the U.S. Environmental Protection Agency. The method, known as the Data Attribute Rating System (DARS), is still in a conceptual stage. The principle behind this approach is to characterize the emission factor and activity data applied in any source category in terms of the underlying attributes that affect those parameters.

Currently, the attribute lists for both the emission factor and activity parameters include a measurement attribute, a source definition attribute, a spatial scale attribute, and a temporal scale attribute. The emission factor may also include a pollutant specific attribute. Each of the attributes is then assigned a score based on a set of criteria. The score for all attributes are then added and the sum is divided by the maximum possible score to define a dimensionless scale value from 0.0 to 1.0, that can be used to compare alternate estimates for a given parameter or to compare the reliability of different parameters in the same inventories. Once the parameter scale values are derived the quality of the overall emissions estimate can be assessed by multiplying the parameter scores for an overall score for the emissions estimate.

Although this approach is still considered a subjective approach, a reasoned selection of attributes and tha acceptance of a defined set of criteria for scoring the individual attributes can provide a more consisetent numerical value to replace the letter scale grading systems used in most other accepted rating systems. This approach offers the potential for a significant breakthrough in emissions inventory verification by providing two important elements. First, the approach can be universally applied to inventories on many scales (source, urban, regional and global), and it is based on a common terminology for the rating of inventories, thereby enhancing the transparancy of the rating system and the rated inventories. The selection of this single approach for a detailed discussion in this appendix is not meant to imply that other rating systems are not useful. Rather, this approach is discussed separately in an attempt to begin a debate within the emissions inventory community in the United States and Europe that will ultimately result in the development of a universal approach that will satisfy the verification needs of a large number of inventory types. The principals of the DARS are outlined in the following discussion.

Description of the Attributes

A discussion of the attributes that affect emissions data quality is presented in the following paragraphs. A suggested scoring scale and a brief discussion of the criteria for selecting a particular score is provided with the discussion of each attribute. It will become apparent to the reader that the application of the suggested criteria and the ultimate scoring of the quality of each attribute retains a subjective nature and that different individuals could easily arrive at different absolute scores for the same attributes and subsequently for the same emissions inventory data. The criteria and attributes are believed to be specific enough, however, to ensure that two individuals would arrive at consistent relative rankings when scoring more than one inventory or more than one approach for developing an emissions estimate for a specific source category.

Measurement Attribute

The measurement attribute is related to the type, quantity and coverage of the measurements that were used to develop the value of the parameter. For example, an emission factor that is based on repeated measurements of a large number of sources covering the range of typical operating conditions is of higher reliability than an emission factor that is based on a single measurement of one source when applied universally to all sources in a given emissions category. Similarly, an emission factor based on a mass balance analysis would typically be considered less reliable than one based on measurement data, and an emission factor based on an engineering assessment would normally be considered even less reliable.

A similar analyses can be completed for the activity data used to develop an emissions estimate. Activity data, such as raw material feed, or fuel consumed, for a specific source that is based on continuous measurement would be of higher quality than an activity estimate based on a related surrogate. For example, an measurement of the amount of fuel consumed in a boiler over a given period of time would be scored higher than a fuel consumption estimate based on a prediction of load demand for a certain process. Another example would be an estimate of mobile source activity based on a measurement of vehicle miles travelled on specific road segments which would be of higher reliability than an estimate based on fuel sales and average miles per gallon or kilometers per liter in the fleet.

One example for the scoring scale for the measurement data attribute that has been suggested is summarized in Table A-1.

TABLE A-1. SUGGESTED SCORING SCALE FOR THE DARS MEASUREMENT ATTRIBUTE

Score	Emission Factor Criteria	Activity Data Criteria
10	Continuous or near continuous measurement of emission rates from all relevant sites; data capture greater than 90%	Direct continuous measurement of raw material feed rate, production rate or consumption rate; data capture greater than 90%
9	Measurement of emission rates from a representative sample of sources over a range of size, and load	Direct intermittent measurement of raw material feed rate, production rate or consumption rate covering a representative sample of sources
5	Emission factor derived from laboratory, bench scale or pilot studies; multiple samples representative of actual process	Activity rate derived from a measured surrogate that has a demonstrated statistical association with the activity causing emissions (e.g., correlation); data covers a representative sample
3	Emission factor based on mass balance, known physical principles or other first principles	Activity rate derived from engineering or physical principles (e.g., design specifications, nominal load demands)
1	Emission factor based on expert judgement	Activity estimate based on expert judgement

Source Definition Attribute

The source definition attribute represents the degree of specificity associated with the application of an emission factor or activity parameter to an individual source category. For example, there are well documented emission factors to represent external combustion boilers that differ slightly for different types of boiler design (e.g., wall fired, overfeed stoker, and traveling grate). These emission factors would receive a high source definition score when applied in an inventory that segregates boilers at that level of specificity. In contrast, an average emission factor developed from an assumed population of boilers expressed in terms of electricity demand would not be scored as high. Another example is represented for the case of a well documented emission factor for CH_4 emissions resulting from enteric fermentation for dairy cattle. When applied to dairy cattle the source specificity for the emission factor would score 10, the same factor applied to all cattle would score 9 or 8, and the same factor applied to all domestic ruminants might score 5 or 6.

Table A-2 presents a suggested scoring schedule for the source definition attribute.

Pollutant Specificity Attribute

The pollutant specific attribute is only applied to the emission factor component of the emission estimate. The methodologies and data sources used to develop activity data are truly unrelated to the choice of pollutants that are represented in inventories. While it is true that in many cases it is desirable to develop emission factors for air toxics or specific components of PM-10 or VOC relative to activity data units that are routinely used in more general emission inventories the origin and development of the emission factors themselves have little relation to the development of the activity data. This attribute is applied to distinguish between emission factors that are developed for specific application to a particular pollutant and an emission factor derived from a surrogate speciation profile applied to a source category or any other indirect application to specific pollutants. Emission factors developed for the specific pollutant will score high, those based on a measured ratio to a common pollutant will be lower and those based on a speciation profile applied to an entire source category will be even lower. A suggested scoring schedule for the pollutant specific attribute is presented in Table A-3.

Spatial Scale Attribute

The spatial scale attribute is used to score the data relative to its reliability for activities and processes in specific regional or urban applications. Spatial variability can affect the quality of emission factors and activity data. In many applications emission factors and activity data are known or estimated at a spatial scale that differs from the spatial scale of the intended inventory. For instance, fuel consumption associated with a particular activity may be measured and well documented at a country-level, or at a State or similar geopolitical unit level. When it is necessary to estimate emissions at a finer level of spatial resolution these aggregate data are often

TABLE A-2. SUGGESTED SCORING SCALE FOR THE DARS SOURCE DEFINITION ATTRIBUTE

Score	Emission Factor Criteria	Activity Data Criteria
10	Emission factor developed specifically for the intended source category or process	Activity data is developed directly for the source of process activity and is expressed in units consistent with the activity and the applied emission factor
9	Emission factor developed for a subset or superset of the intended source or process units and the variability of the factor for the application is low	Activity data representative of a subset or superset of the category with the activity data expressed in similar units
8	Emission factor developed for a similar category with limited variability or a high degree of correlation to intended category or process	Activity representative of a similar category that is highly correlated to the intended category or process
5	Emission factor developed for a subset, superset or similar source category with moderate to high expected variability from the intended source or process	Activity data derived from a subset, superset or similar category with a high variability or low correlation to the intended category
3	Emission factor developed for a surrogate activity with limited information to establish or estimate its degree of correlation to the intended category or process	Activity data representative of a surrogate category with limited information to establish or estimate the degree of correlation to the intended category or process
1	Emission factor developed for a surrogate category and applied to the intended category through engineering or expert judgement	Activity data representative of a surrogate category and applied to the intended category through engineering or expert judgement

TABLE A-3. SUGGESTED SCORING SCALE FOR THE DARS POLLUTANT ATTRIBUTE

Score	Emission Factor Criteria
10	Emission factor developed specifically for the intended pollutant.
8	Emission factor based on a measured ratio to a more commonly measured pollutant that is strongly related to the intended pollutant in that source category.
6	Emission factor based on a representative speciation profile relative to a more commonly measured aggregate pollutant.
3	Emission factor based on a speciation profile for a similar source activity.
1	Emission factor based on a expert judgement or assumption of process conditions and common emission factors.

allocated to the smaller spatial scale by applying some surrogate distribution factor (e.g., population, or employment). Similarly, emission factors are sometimes available for application to one country or region, and later applied to other countries or regions with a different economic base or climate.

Table A-4 presents a suggested scoring schedule for criteria applied to the spatial scale attribute.

Temporal Scale Attribute

This attribute is used to rate the application of the emission factor or activity based on the time scale of the inventory. For example, an emission factor for a certain process that goes through frequent start up and shut down procedures may have an emissions rate that varies considerably through those cycles relative to the emissions rate at steady state production. If an emission factor is based on the annual operating conditions it would be unreliable in those start up and shut down phases. Emission factors and activity data can be affected by seasonal influences, changes between day and night. Activity data can also be dependent on operations for the typical weekday and weekend day. The specific conditions that can affect the temporal variability of emissions data include but are not necessarily limited to temperature, wind speed, solar radiation, humidity, snow and ice ground cover and soil moisture content. Biogenic sources

TABLE A-4. SUGGESTED SCORING SCALE FOR THE DARS SPATIAL SCALE ATTRIBUTE

Score	Emission Factor Criteria	Activity Data Criteria
10	Emission factor is developed for and specific to the activity at the given spatial scale	Activity data are developed for and specific to the geographic region of the inventory
8	Emission factor developed for a spatial scale either smaller of larger than that of the current inventory effort for applications where spatial scale variability is expected to be low	Activity data scaled from a region of either smaller or larger scale, scaling factors are both correlated to the actual activity and representative of the specific geographic area
3	Emission factor developed for a spatial scale either smaller or larger scale and spatial variability large as a result of different relief, climate, economic base or other factor	Activity data representative of either smaller or larger scale and the scaling factors are not correlated well with the activity
1	Emission factor based on unknown spatial scale or is applied to a category with unknown spatial variability	Activity data spatial variability unknown

are also dependent on the stage of the growth cycle. Any factors or activity data that are developed for an average condition or a very specific condition will introduce uncertainty when applied to problems covering different time scales. Table A-5 presents a suggested scoring schedule for the temporal scale attribute.

Application of Date Attribute Rating System

Each attribute is assigned its score based on a set of criteria as suggested in Tables A-1 through A-5. The total scores for the attributes are summed and divided by the maximum score for all attributes to define a numerical score between 0.1 and 1.0. The scores for the emission factor and activity data can then be multiplied to derive an overall inventory ranking. The data can be used to compare different emission factors or activity data and overall inventories.

TABLE A-5. SUGGESTED SCORING SCALE FOR THE DARS TEMPORAL SCALE ATTRIBUTE

Score	Emission Factor Criteria	Activity Data Criteria
10	Emission factor developed for and applicable to the same temporal scale as the inventory	Activity data is specific for the temporal period represented in the inventory
9	Emission factor is developed from an average of repeated measurement periods for the same temporal scale (e.g., for several years covering the same month)	Activity data is representative of the same temporal period but is based on an average over several repeated periods (e.g., activity for the spring but is average of the most recent 3 spring periods)
7	Emission factor derived for a longer or shorter time period, or for a different year or season, but the temporal variability is expected to be low	Activity data representative of a longer or shorter time period or a different year or season but temporal variability is low
3	Emission factor derived for a longer or shorter time period or a different year and the temporal variability is expected to be high	Activity data representative of a longer or shorter time period or a different year, and the temporal variability is expected to be high
1	Emission factor basis difficult to assess in temporal basis or information is lacking to establish temporal variability	Activity data representative of a longer or shorter time period and the temporal variability is difficult to assess

Similarly, each attribute is scored individually so that the components that contribute significantly to the uncertainty can be prioritized. This approach can offer a powerful capability to understand the relative merits of alternate inventories and alternate approaches to developing inventories but can also indicate the specific areas where improvements in understanding of emission factors and/or activity data would have the greatest benefits.

It is important to remember that each attribute must be considered independently to extract the most detail and meaning from the final ranking. This issue could be particularly confusing in relation to the interpretation of the measurement, source definition and pollutant specific attributes. The measurement attribute is intended to assign a quality or reliability estimate solely on the basis of the methods or extent of measurement data used to compile either the emission factor or activity data. The source specific attribute, however, is intended solely to rank the estimate as it applies to the specific source category or group of source categories represented in the inventory. As such, the ranking is unaffected by the absolute accuracy of the emission factor or activity data, or the perceived reliability of the data value. It is only used to assess whether the value used is specific for the particular source category. Similarly, the pollutant specific attribute does not reflect an assessment of the accuracy of the emission factor, but is only related to specificity of that emission factor to the pollutant represented in the inventory.

Therefore, it is entirely possible that an emission factor could receive a high score for the measurement attribute and pollutant specific attribute, but a low score for the source definition attribute. This situation would arise in the case where an emission factor was based on many high quality measurements of the emission rate of the specific pollutant, but those measurements were made on sources that are similar but different from the source being assessed. The appropriate use of this technique, therefore, will require practice and discipline on the part of the researcher.

It is also important to realize that there is a significant amount of subjectivity associated with the application of the technique. When two or more researchers apply this technique to a single inventory or a component of an inventory it is almost certain that the final scores will differ. If the various scorers have a common understanding of the underlying data and the meanings of the attributes and their ranking criteria the differences in final scores should be small. Therefore, analyses based on the application of this technique should not make distinctions relative to the overall reliability of emissions estimates based on scores that differ marginally from one another. When scores differ by 15 percent or more, there should be reason to question the results and review techniques and the inventory development methodologies used in the different estimates. In general, when there are ranges of scores, the inventory with the highest overall score would be favored in terms of its reliability. A strength of this approach, however, allows the review of the sources of the high and low scores and the attributes that contribute to the high and low scores. Therefore, a knowledgeable researcher can make assessments of the importance of each attribute for the particular inventory application and reach conclusions from the proper perspective.

An example of application of DARS

As an example of the application of DARS consider the development of an inventory for VOC emissions resulting from vehicle refueling of gasoline automobiles for one day with an ozone standard exceedence in one county in one State in the United States. The emission factor is estimated using EPA's MOBILE5.0 emission factor model. The source category is specific for refueling activities and the pollutant is specific for VOC from automobiles. The spatial scale attribute was ranked relatively low because the data used are state specific and temperature can vary for counties within a state. Similarly, the temporal scale attribute was ranked intermediate because average summer temperatures are applied to represent the emissions for a specific day.

The fuel consumption activity data is based on gasoline taxes, and although this is a surrogate it is highly correlated with fuel consumption. The tax is collected at the state-level and apportioned to county which decreases the confidence in the county-level estimate, and it is assumed that gasoline sales per day in the summer months are relatively constant. These assumptions are used to generate the analysis summarized in Table A-6.

TABLE A-6. EXAMPLE OF DARS APPLICATION FOR VOC LOSSES FROM REFUELING OF GASOLINE AUTOMOBILES IN ONE NONATTAINMENT COUNTY

Attribute	Attribute Criteria Ratings		
	Emission Factor	Activity Data	Overall Estimate
Measurement	8	7	0.56
Source Specific	10	8	0.80
Pollutant	10	-	1.00
Spatial Scale	7	7	0.49
Temporal Scale	8	9	0.72
Composite	0.86	0.78	0.67

This analysis shows a high degree of confidence in the overall emission estimate with a composite score of 0.67. The major factors that contribute to the high confidence are the pollutant, source definition and temporal scale attributes and the variables for the measurement attribute for the activity data and the spatial scale attribute represent the areas where improvements could be made.

Essentially any emissions estimate could be assessed in this way. At times the specific techniques used in some types of estimates would not coincide directly with the attributes and the criteria suggested in this discussion. One alternative that is under discussion is a system to allow weighting factors to be applied to each attribute. The advantage of adding this feature is that it would allow the researcher to compensate for attributes that are either not applicable or not of an equal importance in specific applications. The disadvantage is that it would add complexity and increase the subjectivity in the analysis. Further work is being completed to refine this approach to develop a more consistent list of attributes and criteria that can be widely applied in a variety of inventory development efforts.

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16. ABSTRACT

This document reports on a study of the concepts and techniques involved in emission inventory development and verification. The study is the result of interaction among the Verification Expert Panel of the Task Force On Emission Inventories, which was sanctioned under the United Nation Economic Commission For Europe. The verification opportunities discussed range from simple approaches to sophisticated modeling and data manipulation techniques that require technology that is yet emerging. The five primary elements of a verification program, as identified by the Panel, are:

- Documentation of Data Quality
- Application of the Data
- Comparison of Alternative Estimates
- Uncertainty Estimates
- Ground Truth Verification

This report discusses geopolitical, budgetary, and time constraints that will affect the quality of emission inventories, and it guides users in selecting appropriate methods for various situations and conditions. The future will require more accurate and flexible emission inventory data and technology, and future efforts will benefit from the application of many of the inventory approaches discussed in this report.

17. KEY WORDS AND DOCUMENT ANALYSIS

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