Quantification of Uncertainty in Emission Factors and Inventories

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ABSTRACT

For both scientific and policy reasons, there is increasing demand for quantification of variability and uncertainty in emission factors and inventories. Variability refers to inherent differences in emissions among different sources or for a given source over time. Uncertainty refers to lack of knowledge regarding the true value of emissions at a given location and time period. Scientific advisory organizations such as the National Academy of Sciences and EPA's Science Advisory Board often call for increased quantification of variability and uncertainty, either directly with respect to emissions or in integrated assessments of which emissions characterization is a component (e.g., human health risk assessment). The Office of Management and Budget has required quantification of uncertainty as part of regulatory impact assessment. EPA's Office of the Inspector General recently released a report specifically calling for quantification of uncertainty in emission factors. Thus, it appears not to be a question of if uncertainty analysis should be done, but rather, how? This paper will provide an overview of methods for and examples of quantification of variability and uncertainty in emissions factors, and quantification of uncertainty in emission inventories, based on an accumulated body of research over a number of years and spanning a variety of emission source categories and pollutants. Furthermore, the implications of several key guidance and advisory documents, such as the Intergovernmental Panel on Climate Change (IPCC) Guidelines for National Greenhouse Gas Emission Inventories and the NARSTO Emission Inventory Assessment, will be briefly summarized. Key findings, conclusions, and recommendations will be offered regarding practical strategies for moving forward in the effort to quantify uncertainties in emissions.

INTRODUCTION

The purpose of this paper is to identify motivations, summarize the current state of practice, identify improved approaches, and make recommendations regarding quantifying variability and uncertainty in emission factors and emission inventories.

THE IMPORTANCE OF EMISSION INVENTORIES TO DECISION-MAKING

Emission inventories are compilations of the contributions of individual source categories to total emissions for one or more pollutants for a given time period and geographic area. Inventories are used for a wide variety of decision making purposes (e.g., NARSTO, 2005; EPA, 2006). Examples include: development of control strategies for reducing emissions; strategy development for emissions permit trading activities under "cap and trade" programs; emissions trends analysis; projections of future emissions; permit limit determination; emission statements for fee collection purposes; international treaty reporting requirements (e.g., for greenhouse gas emissions); environmental impact modeling;

compliance determination; real-time air quality forecasting; exposure and risk analysis; accountability assessments; and prioritization of data needs, among others.

Structure of Emission Inventories
The development of emission inventories must take into account the contributions of many types of emission source categories. These categories are often broadly classified as point (stationary), line (onroad mobile for major highways), and area sources (including onroad mobile on secondary streets, as well as nonroad mobile and nonmobile area sources). An alternative high level classification is with respect to anthropogenic versus "biogenic" sources. The latter may also include non-biological but natural sources such as volcanoes and lightning. This latter distinction is useful in the sense that anthropogenic sources are potentially controllable, since they result from human activity. However, some biogenic sources are influenced by human activity that leads to changes in land-use and vegetation cover (e.g., deforestation).

Emission inventories are developed for a wide variety of pollutants, including primary emissions of gases and particles. However, for some air quality problems, such as ozone or ambient fine particulate matter (PM), there are multiple precursors that undergo transformations in the atmosphere to form the secondary pollutants of interest. Hence, emission inventories are often needed for multiple pollutants in order to assess the combined effect of changes in emissions of several pollutants on ambient levels of ozone and fine PM.

An emission inventory can be expressed as a fairly simple mathematical equation:

Equation 1: $EI = \sum_i \left(EF_i \times AF_i \right)$

where:

EI = Total emission inventory for a given pollutant, geographic area, and time period, typically in units of tons.

EF_i = Emission factor for the emissions of a given pollutant from source category i, in units of mass per unit of activity. An example would be grams of pollutant emitted per gigajoule of energy input to a power plant, or grams of pollutant emitted per vehicle-mile of travel.

AF_i = Activity factor for source category i. Examples would be gigajoules of energy input to power plants or vehicle-miles of travel in a particular geographic area for a particular period of time.

Questions that Decision-Makers Typically Ask Regarding Emission Inventories
Emission inventories are critical to many environmental decision-making processes, as noted earlier. Furthermore, there are specific questions that decision-makers may ask that further motivate the need to deal with uncertainties in emission inventories. The list of questions given here is adapted from a focus group study of senior EPA decision makers who deal with risk management issues (Bloom et al., 1993). These questions may include:

- How well do we know these numbers?
- What is the precision of the estimates?
- Is there a systematic error (bias) in the estimates?
- Are the estimates based upon measurements, modeling, or expert judgment?
- How significant are apparent trends over time?
- How effective are proposed control or management strategies?

- What is the key source of uncertainty in these numbers?
- How can uncertainty be reduced?

In order to answer these questions, one must have some idea of the precision and accuracy of the estimates that comprise an emission inventory. This in turn motivates the need to characterize uncertainty in emission factors, activity factors, and the overall inventory.

Recommendations Regarding Quantification of Uncertainty in Emission Inventories

The National Research Council (NRC) has made numerous recommendations regarding quantification of uncertainty in emissions estimates and emission inventories, including but not limited to the NRC (1991) report on urban and regional air quality, the NRC (1994) report on science and judgment in risk assessment, and the NRC (2000) report on modeling mobile source emissions.

The NARSTO emission inventory assessment has recommended quantitative approaches to uncertainty and sensitivity analysis of emission inventories, and provides an extensive literature and overview of practical methods (NARSTO, 2005).

The Intergovernmental Panel on Climate Change (IPCC) has developed and refined guidance on quantification of uncertainty in national greenhouse gas emission inventories, including the IPCC Good Practice Guidance and Uncertainty Management in National Greenhouse Gas Inventories (IPCC, 2000) and IPCC Guidelines for National Greenhouse Gas Inventories (IPCC, 2006). These guidelines have been developed by representatives of many countries and represent tiered approaches that can be selected according to objectives and resource availability.

A recent report by the EPA Office of the Inspector General makes specific recommendations for how EPA's Office of Air and Radiation (EPA, 2006). These recommendations include development of guidance on "how to account for emissions factors uncertainty in newly developed factors and key existing factors," and development of plans to "ensure emissions factors uncertainty analysis is included in the development, rating, and intended uses of emissions factors."

CURRENT APPROACHES TO CHARACTERIZING UNCERTAINTY IN EMISSION INVENTORIES

Although uncertainties are inherent in and widely acknowledged regarding emission factors, current practice for dealing with uncertainties in emission inventories primarily focuses on qualitative ratings for individual emission factors (EPA, 1995). The qualitative ratings are based on an emission test rating followed by an emission factor rating. The emission test rating considers whether the tests were performed using a sound methodology and are documented adequately to allow for adequate validation. The emission factor rating takes into account the test rating, the number of sources tested, and whether the sources are selected at random, represent the industry population, and are sufficiently specific (e.g., to fuel type, design, etc.) in order to minimize inter-plant variability.

The U.S. EPA Office of Inspector General evaluated trends in the quantity and quality of emission factors that are reported by the U.S. EPA. As of March 1996, there were 8,830 emission factors, of which 27 percent were rated either A or B. As of September 2004, there were 17,110 emission factors, of which 23 percent were rated A or B. Thus, as the number of emission factors increases, the overall quality of the emission factors appears to be decreasing. There are likely reasons for this trend. For example, many of the newer emission factors are for source categories, pollutants, or combinations of both that had previously not been quantified. Thus, one might expect that initially, these new emission factors might tend to be of lower quality than those that have been developed and refined over the years.

Many of the newer emission factors are for fine particulate matter or hazardous air pollutants for which there are significant challenges with respect to obtaining adequate representative samples of measurements, because of factors such as cost, averaging time of the measurements, logistics of field data collection, and limitations of sampling and analytical methods.

In addition to focusing on qualitative ratings of uncertainty in emission factors, there has been limited effort to develop qualitative ratings of entire inventories. One such effort has been the Data Attribute and Rating System (DARS) (EIIP, 1996). DARS uses numerical scores for various attributes of an inventory. The scores are based on subjective assessments. DARS has bee proposed for a wide variety of applications, but it is not clear that it is used in practice.

Some challenges and shortcomings of qualitative rating methods is that they do not enable explicit quantitative comparison of uncertainties for different emission factors or inventories, and they may be inconsistent if judgments regarding ratings or scoring are not applied systematically.

For example, an emission factor rating of A does not clearly convey or imply what the quantitative uncertainty would be regarding an emission factor. As an example, based on a statistical analysis of random sampling error, the uncertainty in the average A-rated emission factor for NO_x emissions from bituminous coal-fired wall-fired, dry-bottom boilers is plus or minus 15 percent relative to an average value of approximately 21 lb NO_x per ton of coal. However, the range of inter-plant variability in these emission factors is approximately a factor of two, ranging from approximately 10 to 45 lb NO_x per ton of coal among 28 plants where measurements were taken. This example illustrates that if an average emission factor is used to estimate emissions for a large sample of sources, the uncertainty in the estimate is much smaller than if the emission factor is used to estimate emissions for an individual source. Thus, the same emission factor can have substantially different ranges of uncertainty depending on how it is used. Of course, while the typical guidance on emission factors is that they should be used only to estimate average emissions for a large number of sources, this is not how they are always used in practice.

SOURCES OF VARIABILITY AND UNCERTAINTY IN EMISSION FACTORS AND EMISSION INVENTORIES

Variability refers to the certainty that different emission sources will have different emissions (inter-unit variability) or that emissions will vary over time for a given source (intra-unit variability). *Uncertainty* refers to lack of knowledge regarding the true value of a fixed but unknown quantity, or the true population distribution for variability. Both variability and uncertainty depend on averaging time. Typically, the variability in short term (e.g., hourly) emissions is much greater than that for long-term (e.g., annual) emissions. Similarly, the uncertainty associated with short term emissions is usually much larger than that associated with long-term estimates.

The most typical sources of intra-unit or inter-unit variability in emissions include:

- Design: differences in the design and configuration of an emission source can lead to differences in factors that influence emissions (e.g., combustor geometry)
- Feedstocks: some emissions depend directly on the concentration of elements in the feedstock, such as sulfur, trace metals, or ash in coal which can lead to emissions of sulfur dioxide, various hazardous air pollutants, and particulate matter, respectively.
- Ambient Conditions: differences in ambient conditions, such as temperature, humidity, and barometric pressure can influence the emissions of some pollutants, such as evaporative volatile

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organic compound (VOC) emissions or nitrogen oxides (NO$_x$) emissions from combustion processes.

- Maintenance Practices: Differences in maintenance practices can lead to variations in the efficiency and emissions of a facility.
- Operational practices and occurrences: Some types of facilities can be operated with particular goals. For example, a power plant would be operated differently if the goal is to maximize thermal efficiency, minimize emission rates, or maximize power output. Operational procedures that maximize power output, for example, can lead to more severe operating conditions, and greater maintenance and repair requirements, that may affect emission rates. Efforts to operate the plant so as to minimize emissions subject to a particular production rate could motivate optimization of fuel-to-air mixing which may or may not enhance thermal efficiency. Another factor that can affect emissions is a process upset.
- Seasonality/Periodicity: Some industries can operate at baseload for extended periods of time, while others may have daily, weekly, or seasonal cycles. The emissions characteristics during transients may be different than those during steady-state operation of a facility.

The typical sources of uncertainty in emission factors and inventories include:

- Random sampling error. This is also sometimes referred to as statistical error and is quantifiable using frequentist statistical methods assuming that data are a random representative sample. For example, this type of error is the basis for estimation of confidence intervals based on the standard error of the mean.
- Measurement errors. Each measurement may contain error because of imperfections in sampling and analytical methods. Measurement errors are typically categorized as systematic and random errors. Systematic errors lead to a bias, in which the average value of repeated measurements does not converge to the true value of the quantity being measured. Random errors lead to imprecision of measurements, such that repeated measurements are randomly distributed above and below the true value. Measurements can have various combinations of bias and imprecision.
- Non-representativeness: This source of uncertainty is difficult to quantify and arises when the specific sources that are tested, or the conditions under which the sources are tested, are not representative of the real world situation that affects emissions for the geographic area and time period of interest. Furthermore, it is possible for a set of data to be representative for one purpose but not for another. For example, if one has data regarding emissions from a random sample of power plants in a particular state during steady state operations in the summer time, such data might be useful for assessments for that same geographic area, time period, and operating condition. However, such data would not be suitable for assessment of emissions during transients for the particular geographic area and time period, nor might it be representative of emissions for other geographic areas or time periods. The use of non-representative data typically leads to biases in emission estimates.
- Averaging time. Emissions data are measured for different averaging times depending on the pollutant. For example, emissions of some gases, such as NO$_x$, SO$_2$, and others, can be measured at short time resolutions and are often reported on an hourly basis if measured using Continuous Emission Monitoring Systems (CEMS). However, measurements of speciated PM$_{2.5}$ emissions might be based on 24 hour integrated filter-based samples. For facilities that do not have CEMS, measurements might be made in a limited duration "stack test" of perhaps one to three days, thereby representing an averaging time of perhaps a few days (depending on how the data are recorded and reported). Many emission inventories are developed on an hourly basis (for air quality modeling), daily basis, or annual basis. If the time period of the inventory does not match the time period of the measurements, then there can be errors of interpolation or extrapolation. Furthermore, for short averaging times, there can be substantial variability. If

data do not exist upon which to quantify hour-to-hour variability (for example), or if hourly patterns in emissions are autocorrelated or subject to periodicity of varying durations, one could obtain misleading inferences regarding estimates of emissions for time periods other than that of the measurement itself. Another example of this is the use of driving cycle data to estimate vehicle emissions, given that driving cycles are highly variable from one trip to another even if average speeds are similar.

- Omissions. Emission inventories are often challenged by lack of data. There are various types of missing data. Sometimes data are missing because of temporary loss of measurement capability, such as for a CEMS. In some cases, statistical methods could be used to impute missing values. Another common form of missing data is a "non-detect," which is a measurement value that is below the detection capability of the instrument. There are various approaches used to impute or assume values associated with non-detects, some of which are statistically rigorous (but not commonly used) and some of which are inherently biased (and more commonly used). Other typical omissions are situations in which emissions data are available for some pollutants for a particular emission source but not others (e.g., total hydrocarbons but not speciated hydrocarbons, or total $PM_{2.5}$ mass but not speciated $PM_{2.5}$).

- Surrogate data. Surrogate data refers to situations in which directly relevant data are not available, but a judgment is made that an analogy can be made for a situation in which data are available. For some of the types of omissions discussed above, one might be able to fill data gaps based on surrogate data. For example, one may be interested in speciated hydrocarbon data for a particular emission source, but only have data for total hydrocarbons. However, speciated hydrocarbons may have been measured for a similar source. An assumption that the speciation profile of one source is applicable to that for another source is a judgment. Such an assumption may introduce biases if the analogy is weak or not appropriate.

- Lack of relevant data. This situation occurs when there are no relevant data and no realistic or meaningful opportunity to use surrogate data. In some cases, it may be possible to do some theoretical bounding analysis if the pollutant is based on a conserved species (e.g., conversion of a trace species in a fuel to an air pollutant). However, in other cases, such as the formation of organics during a combustion process, a bounding assumption may be difficult to make. These situations can lead to gaps in the inventory, which in turn lead to biases in the inventory. Specifically, the total emissions would be underestimated if there is a lack of data or information upon which to base an estimate for a particular source category. In some cases, it may be possible to use other methods to assess whether the lack of data may be a significant concern. For example, comparison of ambient monitoring data to emission inventory data might help identify biases in the inventory, and therefore assess whether there might be significant unquantified emissions.

METHODS FOR QUANTIFYING UNCERTAINTY: "BOTTOM-UP" APPROACHES

As noted in the introduction, qualitative methods based on emission factor ratings have been widely used, and scoring methods for emission inventories have been proposed (e.g., DARS). However, many scientific organizations, such as the NRC, have recommended that quantitative approaches be used. Such recommendations have been reiterated by EPA's Office of the Inspector General. Here, we briefly review quantitative methods for dealing with uncertainty in emission inventories. More detail on these methods is available elsewhere, most notably NARSTO (2005), IPCC (2006), Morgan and Henrion (1990), Cullen and Frey (1999), and various peer reviewed journal papers that are cited in the text below. The methods reviewed here are referred to as "bottom-up" approaches because they involve quantifying uncertainties in individual inputs to an inventory, and combining the input uncertainties to estimate their joint effect on uncertainty in the total inventory.

Figure 1. Conceptual Diagram of Estimation of Uncertainty in a Total Emission Inventory for a Given Pollutant, Geographic Area, and Time Period based on Uncertainties in Emission Factors and Activity Factors.

Input Uncertainties

Source Category	Emission Factor	Activity Factor
1		
2		
k		

Emission Inventory

Output Uncertainty

Total Emissions
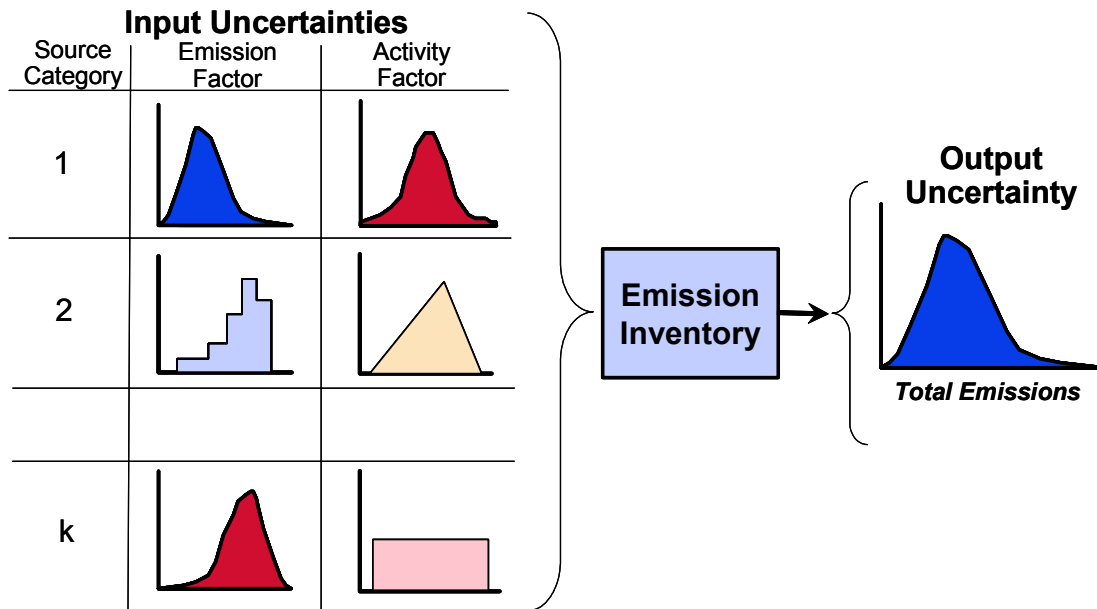
Probability is a natural language for describing uncertainties, and offers advantages of a consistent axiomatic foundation, a variety of methods for estimating uncertainties, and a variety of methods for communicating and analyzing uncertainties. A conceptual diagram of estimation of uncertainty in an inventory based on uncertainties in the inputs to an inventory is shown in Figure 1.

While there are nonprobabilistic methods for dealing with uncertainties in emission factors and inventories, these are not emphasized here for several reasons. Non-probabilistic methods can include interval analysis and fuzzy numbers, as examples. Interval analysis is a useful way to place bounds on the assessment. However, when the bounds are very wide, the analysis can become uninformative. Fuzzy numbers are used in many applications. However, fuzzy numbers represent vagueness, rather than uncertainty. Thus, the interpretation of fuzzy-based results for purposes of decision making appears to be a challenge.

As noted in NARSTO (2005), quantitative methods typically involve specifying probability distributions for inputs to an inventory, and propagating the distributions through the inventory in order to estimate the distribution of uncertainty for the total inventory. Distribution assumptions regarding inventory inputs can be developed based on empirical data, encoding of expert judgment, or some combination of both. In situations where representative empirical data are available, it may be possible or appropriate to use "frequentist" statistical techniques to fit probability distribution models (e.g., normal, lognormal, etc.) to the available data (e.g., Cullen and Frey, 1999). Frequentist methods can be either parametric or nonparametric.

However, when relevant data are not available, then the direct use of available data can lead to biases in the assessment. An alternative for this kind of situation is to use a "Bayesian" approach to statistical estimation, in which both data and expert judgment can be combined. As the amount of representative data increases, the results obtained from Bayesian methods will asymptotically approach those of frequentist methods. Expert judgments can be encoded using formal elicitation protocols that attempt to

counteract some typical heuristics used by people when formulating judgments that can lead to biases (e.g., Morgan and Henrion, 1990).

Quantitative probabilistic methods for characterizing the combined effect of uncertainties in inputs on the output of a model or inventory range from simple analytical calculations that may be applicable in some situations to more broadly applicable numerical methods such as Monte Carlo methods and bootstrap simulation. Analytical methods are attractive because in some cases they can provide an exact solution. For example, the sum of normal distributions is normally distributed, and the product of lognormal distributions is lognormally distributed. Furthermore, the parameters of the distributions of the sum or product can be estimated based on the parameters of the individual inputs. However, the accuracy and simplicity of analytical methods tends to diminish as the complexity of the assessment increases. For example, because an emission inventory typically includes both multiplicative terms (e.g., emission and activity factors multiplied for an individual source category) and addition (e.g., summation of emissions among individual source categories), the result for the total uncertainty in the inventory may not be exactly normal or lognormal. If the ranges of uncertainty are small, then analytical methods can be used with acceptable accuracy (e.g., IPCC, 2006). However, if the ranges of uncertainty are large, then analytical methods can produce errors. Such errors can, in principle, be corrected. However, as the complexity of the method increases, the use of numerical methods such as Monte Carlo simulation becomes a more attractive alternative.

Monte Carlo methods have the advantage of being able to accommodate a wide range of probability distribution models for inputs to an inventory, including non-parametric empirical distributions and a variety of parametric probability distributions (e.g., normal, lognormal, gamma, Weibull, and others). Monte Carlo methods can be used to generate pseudo-random values from each uncertain model input to estimate an alternative realization of the model output. In this case, the model is the emission inventory (e.g., Equation 1). Monte Carlo methods can be used with a wide variety of models that have different functional forms and complexity (e.g., Cullen and Frey, 1999).

Monte Carlo methods can be applied or adapted to deal with various issues that are often inherent in emission factor data sets, such as: (a) cases in which data may have both lower and upper bounds; (b) the existence of measurements for which results were below the detection limit of the sampling and analytical procedures; or (c) the existence of mixtures of different types of data within one data set. For example, Frey and Burmaster (1999) illustrate and compare the effect of interindividual variability and uncertainty for situations in which data may not have a partical upper bound (e.g., an ambient concentration) versus in which they are bounded (e.g., a partitioning factor). Zhao and Frey (2004a) review conventional methods for dealing with non-detected measurements, which typically lead to biases in estimates of mean emission factors, and propose an asymptotically unbiased alternative method based on maximum likelihood estimation and boostratp simulation. Zheng and Frey (2004) evaluate and recommend methods for dealing with mixtures of data, such as when an emission factor data set includes subgroups that cannot be separated because of lack of explanatory data. Zheng and Frey (2005) evaluate and recommend methods for separating the contribution of measurement error to the estimated inter-unit variability in emission factors. Frey and Rhodes (1998) evaluate the implications of alternative choices of parametric distributions on key statistics of a probabilistic model output, particularly when quantifying both variability and uncertainty.

Guidelines for quantification of uncertainty in emission inventories have not been developed at the national scale in the U.S. However, the U.S. EPA has developed guidelines for probabilistic analysis in the context of human exposure assessment (e.g., EPA, 1997). Furthermore, the Intergovernmental Panel on Climate Change has developed guidance for quantification of uncertainty in national greenhouse gas emission inventories (IPCC, 2006). This guidance incorporates methods for dealing with empirical data,

methods for encoding expert judgment, and methods for propagating uncertainty in inventory inputs to estimate uncertainty in the total inventory.

There have been numerous applications of probabilistic approaches to quantification of uncertainty in emission factors and emission inventories. For example, Frey and Bammi (2002, 2003), Frey and Li (2003), Frey and Zheng (2002b), Zhao and Frey (2004a; 2006) quantified variability and uncertainty in emission factors for a variety of emission source categories, such as: lawn and garden equipment; construction, farm, and industrial equipment; large stationary natural gas-fired internal combustion engines; onroad motor vehicles; and a variety of combustion-based sources. Frey et al. (2002b) and Frey (2003) evaluated approaches for quantifying uncertainty with respect to development of EPA's "MOVES" vehicle emissions model. Uncertainties in emissions can also be quantified using process engineering models, such as regarding the partitioning of hazardous air pollutants through a coal-fired power plant (e.g., Frey and Rhodes, 1996). Examples of the quantification of uncertainty in emission inventories include estimation of uncertainty in utility NO_x emissions (e.g., Abdel-Aziz and Frey, 2003c; Frey and Zheng, 2002a) and in inventories of hazardous air pollutants (e.g., Frey and Zhao, 2004; Zhao and Frey, 2004b). The implications of uncertainties in emission inventories with respect to uncertainty in air quality has been evaluated in various example studies, such as Hanna et al. (2001) and Abdel-Aziz and Frey (2004). NARSTO (2005) provides a more extensive literature review of methods and applications of probabilistic analysis for emission factors, emission inventories, and the effect of emissions uncertainties on estimates of ambient air quality.

A criticism often aimed at the use of probabilistic methods is that they require knowledge or assumptions not only regarding the form of probability distributions for individual inputs to an assessment, but also regarding the dependencies among two more distributions. While it is true that, in some cases, a dependence or correlation can have a significant effect on the assessment output, it is also true that such dependencies or correlations do not matter in many cases. Furthermore, there are ways to deal with these situations. These include various methods for simulating correlations among probability distributions or sensitivity analyses to determine whether such correlations might significantly affect the assessment results (Cullen and Frey, 1999). Abdel-Aziz and Frey (2003a,b,c; 2004) quantified uncertainty in hourly NO_x emissions of individual coal-fired power plant units, taking into account both temporal and spatial correlations using vector autoregressive time series models, and evaluated the implications of these uncertainties with respect to estimated levels of ambient ozone.

The range of uncertainty in emission factors typically varies from approximately plus or minus 10 percent to more than a factor of two, depending on the emission source, pollutant, and averaging time. The uncertainty in total emission inventories likewise varies depending on the pollutant and averaging time. For example, the uncertainty in chromium emissions for Houston, TX was estimated at -20 percent to +34 percent, whereas the uncertainty in arsenic emissions for Jacksonville, FL was estimated at -83 percent to +240 percent.

Sensitivity analysis can be applied in combination with Monte Carlo analysis to identify which inputs to an assessment contribute the most to the overall uncertainty in the results. Mokhtari and Frey (2005) provide guidance regarding the selection, application, and interpretation of sensitivity analysis methods. Frey and Rhodes (1996) used sensitivity analysis to identify which inputs to a process engineering model were most highly associated with both variability and uncertainty in the estimated hazardous air pollutant emissions of a coal-fired power plant. Frey and Zheng (2002a) used sensitivity analysis to determine which types of coal-fired power plants were most highly associated with uncertainty in a statewide NO_x emission inventory. Adbel-Aziz and Frey (2004) used sensitivity analysis to identify which upwind power plant was mostly highly associated with uncertainty in estimated ambient ozone levels. Frey and Zhao (2004) used sensitivity analysis to identify the emission source categories that were most highly associated with uncertainty in urban scale emission inventories of several selected

Figure 2. Example of a Screen Capture from the Analysis of Uncertainty and Variability in Emissions Estimation (AUVEE) Prototype Software Tool. The Example Depicts Uncertainty in a NO_x Emission Inventory for Power Plants for a Six Month Period for a Particular Geographic Area.
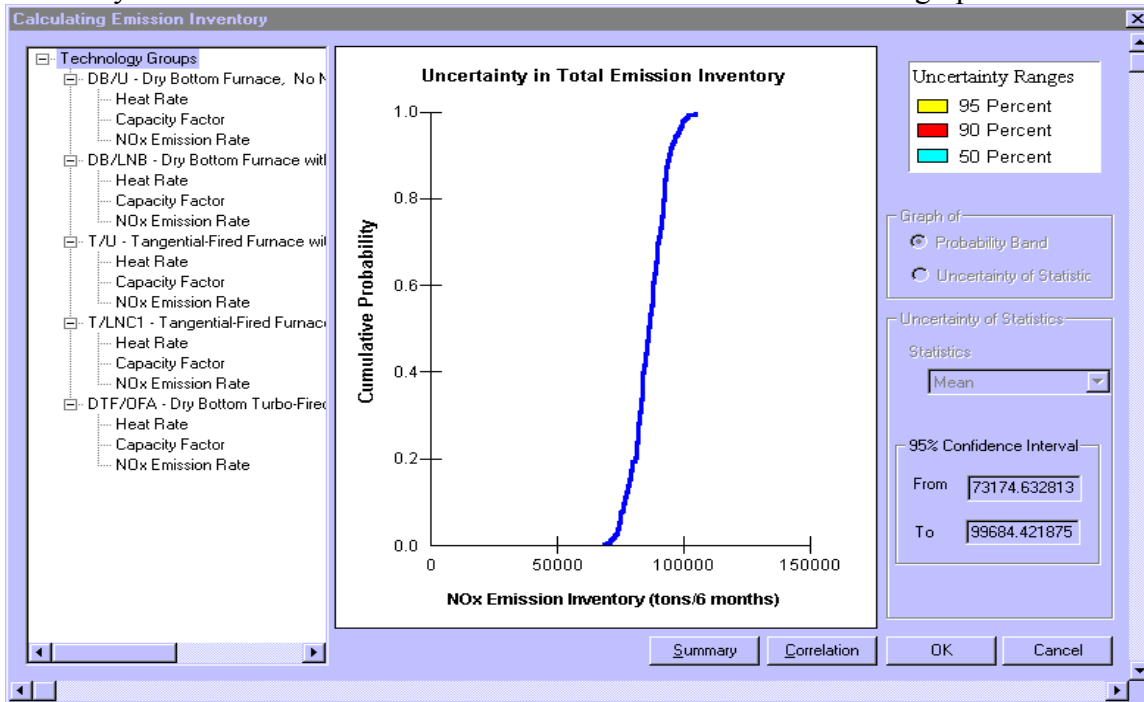
hazardous air pollutants. Knowledge of key sources of uncertainty can help focus data collection or research in order to develop improved estimates of emissions. Knowledge of key sources of variability in emissions can be used to prioritize strategies for controlling emissions. For example, in some cases, only a small proportion of emission sources may contribute substantially to total emissions, or only a few key process plant parameters (e.g., collection efficiency in a control device) significantly affect emission rates.

A prototype software tool was developed for the U.S. Environmental Protection Agency in order to demonstrate a methodological approach for developing probabilistic emission inventories (Frey and Zheng, 2000; 2002a). The prototype software is referred to as Analysis of Uncertainty and Variability in Emissions Estimation (AUVEE). AUVEE includes a graphical user interface (GUI). The software tool allows a user to quantify inter-unit variability in emission and activity factors for selected coal-fired power plant technology groups based on fitting parametric probability distributions to data and the use of bootstrap simulation to quantify uncertainty in key statistics of the fitted distributions (e.g., for the mean emission factor). The user can configure an emission inventory based on entering basic data regarding the size and capacity factor of each power plant unit to be included in the inventory. The software uses Monte Carlo simulation to generate alternative realizations of the inventory, which are characterized as a cumulative distribution function. Sensitivity analysis is used to identify the key sources of uncertainty in the total inventory when comparing the technology groups that comprise the inventory. An example of a screen capture from the GUI of AUVEE is shown in Figure 2. This example illustrates uncertainty in a state-level emission inventory for a six month period that is inclusive of summer months.

A related software tool, AuvTool, was developed for the U.S. Environmental Protection Agency in order to analyze a user-supplied dataset for purposes of fitting nonparametric or parametric probability distribution models for variability and estimating uncertainty in key statistics of the distributions using bootstrap simulation (Frey et al., 2002a; Zheng and Frey, 2002). AuvTool has been used to analyze data

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for emission factors.   AuvTool has more generalized capabilities than does AUVEE for importing data and analyzing variability and uncertainty in individual data sets.

METHODS FOR QUANTIFYING UNCERTAINTY: "TOP-DOWN" APPROACHES

While bottom-up methods are useful for quantifying the precision or random component of uncertainty in an emission inventory, it can be difficult to assess biases. In contrast, top-down methods are useful for assessing biases in an inventory but may not be as suitable for estimating the precision of the inventory. Examples of top-down methods include: (a) comparison of inventories developed using independent methods and data; (b) comparison of air quality model predictions based on inventories to monitored ambient data; (c) comparison of source-oriented versus receptor-oriented air quality modeling approaches; and (d) comparison of inventories and ambient monitoring data. These methods are discussed in detail in NARSTO (2005).

An example of the comparison of inventories developed using independent methods and data is mileage-versus fuel-based mobile source inventories. Most typically, onroad vehicle emission inventories are estimated using gram per mile emission factors obtained from the MOBILE6 model multiplied by estimated vehicle miles traveled by vehicle categories for a given geographic area and time period. This approach is typically based on dynamometer-based vehicle emissions measurements and transportation demand modeling. In contrast, fuel-based emission factors (grams of pollutant per gallon of fuel consumed) can be inferred from remote sensing of vehicle exhaust. Fuel consumption data can be obtained or inferred from county tax records. The fuel-based emission factors can be multiplied by estimated fuel consumption to arrive at a regional total for a given time period. Thus, the mileage-based and fuel-based approaches can potentially use independent data. A comparison of these can identify whether there are substantial disagreements, which may imply that one or both approaches is biased. Of course, while agreement in the results of the two approaches does not guarantee that either is producing a correct answer, the confidence in the answer is increased when there is concurrence.

As an example of the comparison of emission inventories and ambient monitoring data, comparisons have been made regarding the national emission inventories for CO versus the U.S. mean ambient CO concentration (NARSTO, 2005). These trends are very similar. Another typical method for comparing inventories and ambient data is to compare ratios of pollutants. Of course, the comparisons must take into account that pollutants may be undergoing physical or chemical transformations in the atmosphere, such that the ambient trends or ratios may not be the same as for the inventory.

UNCERTAINTY IN EMISSION FACTORS AND INVENTORIES: KEY FINDINGS

Based on research and analysis as summarized in the preceeding sections, several key findings regarding uncertainty in emission factors and inventories have been made. These are summarized below.
- Visualization of data used to develop an inventory is highly informative to choices of empirical or parametric distribution models for quantification of variability or uncertainty.
- Uncertainty estimates might be sensitive to the choice of parametric distribution models if there is variation in the goodness-of-fit among the alternatives. However, in such cases, there is typically a preferred best fit. When several alternative models provide equivalent fits, results are often not sensitive to the choice of the model, unless one is concerned with the tails of the distribution.
- It is not necessary to have large data sets in order to characterize uncertainty. The consequence of small data sets is that uncertainty ranges are larger, if all else is similar. However, a key factor in interpreting any data set is whether it is a random, representative sample. If it is not, then attempts to correct for bias should be considered, including the use of encoded expert judgment.

- A key difficulty in developing probabilistic emission factors inventories is to find the original data used by EPA and others to develop the original deterministic (point-estimate) emission factor.
  - When data are found, they are typically poorly documented.
  - The time required to assemble databases when original data could not be found was substantial.
  - The time to do uncertainty analysis is much shorter if done as part of inventory development.
- Test methods used for some emission sources are not representative of real world operation, implying the need for real world data and/or expert judgment when estimating uncertainty. Examples include some driving or test cycles used for onroad or nonroad vehicles, as well as measurements made at nonrepresentative conditions for stationary sources (e.g., steady-state tests would not capture the effect of transients on emissions).
- Uncertainty in measurement methods is not adequately reported. There is a need for more systematic reporting of the precision and accuracy of measurement or test methods.
- Uncertainties in emission factors are typically positively skewed, unless the uncertainties are relatively small (e.g., less than about plus or minus 30 percent).
- The quantifiable portion of uncertainty attributable to random sampling error can be large and should be accounted for when using emission factors and inventories.
- The range of variability and uncertainty is typically much greater as the averaging time decreases.
- Even for sources with continuous emissions monitoring data, there is uncertainty regarding predictions of future emissions that can be informed by analysis of historical data.
- Prototype software demonstrates the feasibility of increasing the convenience of performing probabilistic analysis.
- Uncertainties in total inventories are often attributable to just a few key emission sources.

CONCLUSIONS AND RECOMMENDATIONS

Based on the findings of the previous section, the following conclusions and recommendations are made:

- Uncertainty and sensitivity analysis should be used to answer key decision maker and stakeholder questions, e.g.,:
  - prioritize scarce resources toward additional research or data collection
  - make choices among alternatives in the face of uncertainty,
  - evaluate trends over time, and so on.
- Uncertainty and sensitivity analysis should be included as functional requirements of an emission inventory from the beginning and incorporated into model and input data development.
- There should be minimum reporting requirements for uncertainty in data (e.g., summary statistics such as mean, standard deviation, sample size).
- There is a need for flexibility in methods for quantifying variability and uncertainty in emission inventories, and identifying key sources of variability and uncertainty, since there are many possible approaches to analysis of uncertainty and sensitivity. Specific choices should be appropriate to assessment objectives, which are typically context-specific.
- Human resources for modeling, including uncertainty and sensitivity analysis, should be appropriately committed.
  - Adequate time and budget to do the job right the first time (could save time and money in the long run);
  - Adequate training and peer review; and
  - Promote workshops and other training opportunities, and periodic refinement of authoritative compilations of techniques and recommended practice.

- Software tools substantially facilitate both uncertainty and sensitivity analysis – there is a long-term need for development of software tools appropriate to specific types of applications for quantifying variability and uncertainty in emission inventories and for evaluating sensitivity of the inventory to variability and uncertainty in its inputs.
- Some areas need more research, investigation, and guidelines, such as identification and evaluation of preferred techniques for communication, and assessment of the real-world information needs of decision makers.
- A multi-disciplinary compilation of relevant case studies and insights from them is a useful way to help convince others of the value of doing uncertainty and sensitivity analysis.
- Uncertainty and sensitivity analysis should be an open and transparent process that is subject to scrutiny and peer review.

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