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Method for Development of Probabilistic Emission Inventories: Example Case Study for Utility NO_x Emissions

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ABSTRACT

Advances in methodology and computing power enable the application of a quantitative approach to characterizing both variability and uncertainty in emission factors. Variability refers to actual differences in emissions from one source to another due to differences in feedstock composition, design, maintenance, and operation. Uncertainty refers to lack of knowledge regarding the true emissions because of measurement errors (both random and systematic), limited sample sizes (statistical random sampling error), and non-representativeness (which can introduce additional errors, including systematic errors). The set of numerical methods generically known as bootstrap simulation are a powerful tool for characterization of both variability and random sampling error. In this paper, we demonstrate the use of bootstrap simulation and related techniques for the quantification of variability and uncertainty for a selected example of NO_x emissions from coal-fired power plants. We have developed a prototype software tool that enables a user to display data sets for emission factors and activity factors for selected power plant technology groups. The user can select a parametric distribution to fit to the data. The user enters information regarding the number of power plant units in the inventory, and can display a variety of results regarding both variability and uncertainty in the inputs to the inventory, as well as uncertainty in various outputs of the inventory. While our example is focused upon emission factors for a selected criteria pollutant, the same methodology can be applied to other pollutants (e.g., hazardous air pollutants, greenhouse gases). The policy relevance of probabilistic inventories will be discussed.

Keywords: Variability, Uncertainty, Emission Inventories, Emission Factors, Activity Factors, Monte Carlo simulation, probabilistic modeling, bootstrap simulation, nitrogen oxides, power plants, data quality, quality assurance

INTRODUCTION

Emission inventories (EIs) are used at federal, state, and local governments and by private corporations for: (a) characterization of temporal emission trends; (b) emissions budgeting for regulatory and compliance purposes; and (c) prediction of ambient pollutant concentrations using air quality models. If random errors and biases in the EIs are not quantified, they can lead to erroneous conclusions regarding trends in emissions, source apportionment, compliance, and the relationship between emissions and ambient air quality.[1]

The National Research Council has recently recommended that quantifiable uncertainties be addressed in estimating mobile source emission factors, and in the past has addressed the need for understanding of uncertainties in emission inventories used in air quality modeling and in risk assessment.[2,3] The U.S. Environmental Protection Agency (EPA) has developed guidelines for Monte Carlo analysis of uncertainty, and has also sponsored several workshops regarding probabilistic analysis.[4,5,6] Probabilistic techniques have recently been applied to estimation of uncertainty in emission factors for mobile sources, major stationary sources and area sources.[1,7-18]

Both variability and uncertainty should be taken into account in the process of developing a probabilistic emission inventory. Variability is the heterogeneity of values with respect to time, space, or a population. Variability in emissions arises from factors such as: (a) variation in feedstock (e.g., fuel) compositions; (b) inter-plant variability in design, operation, and maintenance; and (c) intra-plant variability in operation and maintenance. Uncertainty arises due to lack of knowledge regarding the true value of a quantity. It refers to statistical sampling error, measurement errors, and systematic errors. In most cases, emissions estimates are both variable and uncertain. Therefore, we employ a methodology for simultaneous characterization of both variability and uncertainty based upon previous work in emissions estimation, exposure assessment, and risk assessment.[1,9,10,12-17] The method features the use of Monte Carlo and bootstrap simulation. The approach is illustrated by example for the case of emissions of NO_x from electric utility power plants. The example is conveyed via the Analysis of Uncertainty and Variability in Emissions Estimation (AUVEE) prototype software tool that has been developed for proof-of-concept purposes. The specifics of the methodology used by the AUVEE software are documented in Frey and Zheng.[19] A previous report by Frey, Bharvirkar, and Zheng illustrates the application of similar methods to three case studies.[1]

The purposes of this paper are: (1) to introduce the development of database used in the AUVEE; (2) to introduce some aspects of the development and implementation of the AUVEE system; and (3) to illustrate the methodology developed in this paper by using an example case study from electricity utility power plant NO_x emissions.

GEENRAL APPROACH

The general approach employed to quantify variability and uncertainty in emission inventories and emission factors can be summarized as the following major steps:[19]

1. Compilation and evaluation of a database for emission and activity factors;
2. Visualization of data by developing empirical cumulative distribution functions for individual activity and emission factors;
3. Fitting, evaluation, and selection of alternative parametric probability distribution models for representing variability in activity data and emission factor data;
4. Characterization of uncertainty in the distributions for variability;
5. Propagation of uncertainty and variability in activity and emissions factors to estimate uncertainty in facility-specific emissions and/or total emissions from a population of emission sources; and
6. Calculation of importance of sources of uncertainty via sensitivity analysis.

The details for Step 2 through Step 6 are documented in the Frey, Zheng.[19, 20] The relevant issues for Step 1 are illustrated below through the introduction of the development of database used in the example for the case of emissions of NO_x from electric utility power plants.

DEVELOPMENT OF A DATABASE

In this section, the development of the database used in the case of emissions of NO_x from electric utility power plants and AUVEE is introduced. The data used for the case study is based upon Continuous Emission Monitoring (CEM) for individual power plant units obtained through the U.S. Environmental Protection Agency. In this project, only quarterly data files were used. In the case studies of this project, two averaging times were considered: (1) 6-month; and (2) 12-month. The purpose of the 6-month averaging time was to characterize emissions that include the "ozone season." The purpose of the 12-month averaging time was to be able to characterize annual emissions for emissions budgeting and other purposes.

The 6-month time period is intended to be inclusive of summer months. Therefore, the 6-month averages are based upon combining data from the 2nd and 3rd quarters of the year, including the months from April through September. The 12-month averages are based upon the entire year. At the time that the data collection effort was made, quarterly data were available for the 1st quarter of 1997 through the 2nd quarter of 1999. Therefore, complete datasets of four quarters were available only for 1997 and 1998. Furthermore, data sets needed to characterize the 6-month period inclusive of the summer were available only for 1997 and 1998.

After the data combination and screening processes were completed, the final database was ready for statistical analysis. The data base contains unit/stack identification (unit ID and ORISPL identifier), general information (state, region), technology group (boiler type, NO_x control technology), operation data (capacity, operating time), and ten quarters of NO_x emission data. This database was used as a basis for the internal database of the prototype AUVEE software.

For a power plant unit, emission factors are often reported as mass of pollutant produced per unit of fuel consumed. The unit electrical generation and the power plant efficiency were used to calculate the fuel input. Unit efficiency is typically reported as a "heat rate", which is the ratio of fuel input with respect to electricity generation, in units of BTU of fuel input per kWh of electricity generated. Unit load is often summarized using the capacity factor.

Four quantities were calculated from the combined database. These are: (1) unit/stack heat rate (BTU/kWh); (2) unit/stack capacity factor (actual kWh generated/maximum possible kWh); (3) NO_x emission rate on a fuel input basis (g/GJ); and NO_x emission rate on an energy output basis (g/GJ). Data from the final database was used to calculate the average emission factors and activity factors for each unit or stack and for both averaging times.

The emissions and activity data were calculated for selected technology groups. Four of the technology groups were selected based upon the most prevalent types of units in the data base. These include: (1) dry bottom, wall-fired boilers with no NO_x control; (2) dry bottom, wall-fired boilers with low NO_x burners (LNB); (3) tangential-fired boilers no NO_x controls; and (4) tangential-fired boilers with low NO_x burners and overfire air option 1, referred to as LNC1. The number of data points for these four technology groups ranges from 36 to 136, depending upon the technology group and the averaging time used. In addition, one other technology group was selected that has a small sample size. The reason for selecting this group was to demonstrate that the probabilistic method for developing estimates of variability and uncertainty in emission inventories is able to deal with small data sets. The category for dry bottom, turbo-fired boilers with overfire air has only six data points. The methods used to characterize variability and uncertainty in the emissions associated with these five technology groups can be extended later to include other technology groups.

To simplify the database as much as possible, it is desirable to be able to select data for one representative year. Data for 1997 and 1998 were compared to identify similarities and differences between them. The data for the two years were similar, implying that data for either year could be used as the basis for analysis. The more recent 1998 data were selected. In addition, possible dependencies between activity and emission factors were evaluated. No significant dependencies were found. Therefore, it was not necessary to attempt to simulate statistical dependencies among emission and activity factors.

AUVEE SYSTEM DEVELOPMENT AND IMPLEMENTATION

Here, we briefly introduce the functional design of AUVEE, the composition of the main modules and the relationships among them. In AUVEE, the user sets up a project. The project contains information on the choice of an internal emission factor and activity factors database, project name, project comments, and user data regarding the number of power plant units included in the inventory, the boiler and emissions control technology for each unit, and the capacity of each unit.

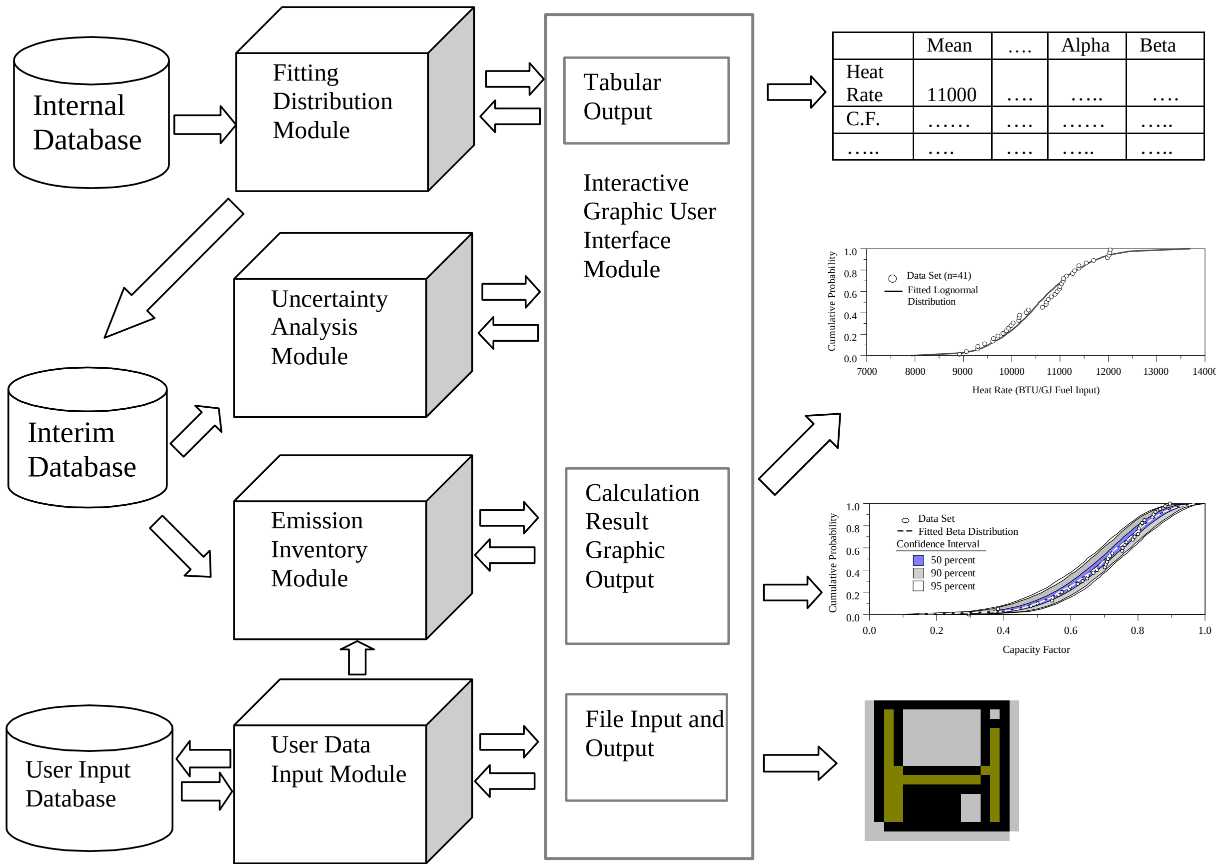
Figure 1 shows the conceptual design of AUVEE. AUVEE is composed of 3 databases, which include an internal database, a user input database and an interim database. In addition, AUVEE includes four main modules: (1) fitting distributions; (2) characterizing uncertainty; (3) calculating emission inventories; and (4) user data input. AUVEE features an interactive Graphical User Interface (GUI).

The user may select either a 6-month average or a 12-month average database as the basis for developing either a 6-month or 12-month emission inventory, respectively. The internal database cannot be modified by the user in the prototype version of the software. The user input database stores data that the user provides regarding the number of power plant units, the boiler and emission control technology for each unit, and the capacity of each unit. This database can be edited by the user via the user data input module.

The interim database in AUVEE is used to store the results from the fitting distribution module and to store project information. A default interim database is provided so that the user can proceed to calculate emission inventory results even without making a new selection of parametric distributions to represent each input to the emission inventory.

The fitting distribution module implements all calculations for fitting parametric distributions to emission factor and activity factor data. This module provides graphs comparing fitted distributions to the data, allowing the user to evaluate the goodness of fit of parametric distributions. The user has the option, via a pull-down menu, to select alternative

Figure 1. Conceptual Design of the Analysis of Uncertainty and Variability in Emissions Inventories (AUVEE) Prototype Software System



parametric distributions for fit to the data. When the user exits the fitting distribution model, the current set of fitted distributions are saved to the interim database for use by other modules in the program.

The characterizing uncertainty module implements the function of characterizing uncertainty in emission factors or activity factors based upon the database and based upon the number of units of each technology group that are in the internal database. The characterizing uncertainty module uses data from the interim database to get distribution information including distribution type and the parameters of the fitted distributions for emission and activity factors. Uncertainty estimates of the mean emission and activity factors, and other statistics, are calculated using the numerical method of bootstrap simulation. The results of the uncertainty analysis are displayed in the GUI. Because this module uses data from the internal database, which may contain a relatively large number of power plant units compared to an individual state emission inventory, the estimates of uncertainty in the mean and in other statistics are typically a lower bound on the range of uncertainty in the same statistic applicable to an emission inventory that includes a smaller number of power plant units.

The emission inventory module has the following functions: (1) it allows the user to visit the user database and append, modify or delete user input data; (2) it characterizes the uncertainty in emission factors and activity factors based on user project data; (3) it calculates uncertainty in the emission inventory; and (4) it calculates the key sources of uncertainty from among the different technology groups. The estimates of uncertainty in the emission inventory module are based upon the number of power plant units of each technology group specified by the user. For example, although there may be 36 power plant units of a given type in the internal database, the user may have only 10 units of that type in the emission inventory of interest. The uncertainty in the emission and activity factors for that technology group will be estimated based upon a sample size of 10, not 36.

The GUI is a general control module in AUVEE, and it makes all independent modules, platforms and databases work together. In addition, the GUI is a bridge which links user input to internal implementation within AUVEE, and provides model output to the user. Through the GUI, the user can build or open a project, enter a database of emission sources, implement user's choice of parametric distributions, view or save all calculation results, and manage the message passing between the different modules.

CASE STUDY: A PROBABILISTIC EMISSION INVENTORY FOR A SINGLE STATE

The case study is based on the number of units of each technology group in a single state. The specific case study was selected because the number of units representing each of four power plant technologies is dissimilar. Specifically, the following numbers of units are included in the case study:

- 19 tangential-fired boilers with no NO_x controls (T/U)
- 11 tangential-fired boilers using Low NOx Burners and overfire air option 1(T/LNC1)
- 12 dry bottom wall-fired boilers with no NO_x controls (DB/U)
- 3 dry bottom wall-fired boilers using low NO_x burners (DB/LNB)

No units of the technology group with dry bottom turbo-fired boilers and overfire air are present in the example state. The case study is based upon a 6-month period. Parametric probability distributions were fit to each activity and emission factor required for the inventory. The results are summarized in Table 1, estimated by AUVEE using Maximum Likelihood Estimation (MLE). Examples of the fitted distributions for the example of one technology group are shown in Figures 2, 3, and 4 for an emission factor, a capacity factor, and a heat rate, respectively. The goodness-of-fit was evaluated by comparing confidence intervals of the fitted distribution, obtained from bootstrap simulation, with the data. For example, the lognormal distribution fitted to the heat rate data agrees well with the tails of the distribution of the data. There are some deviations of the fitted distribution from the data in the regions of the 40th to 70th percentiles. However, more than half of the data are enclosed by the 50 percent confidence interval and almost 100 percent of the data are enclosed by the 95 percent confidence interval. On average it is expected that 95 percent of the data should be enclosed by the 95 percent confidence interval if the data are consistent with the assumed probability distribution model, and some random variation of this percentage is also expected. Therefore, in this case, the fitted distribution is deemed to be an adequate match with the data.

Table 1. Summary of 6-Month NO_x Emission and Activity Factors and of Fitted Distributions for Five Power Plant Technology Groups

Technology Group	Input Variables	Summary of Data			Fitted Distributions		
		No. of Data Points	Mean	Standard Deviation	Dist. Type	1st Para.*	2nd Para.*
DB/U	Heat Rate	87	11,190	1,440	Lognormal	9.31	0.122
DB/U	Capacity Factor	87	0.59	0.18	Beta	3.92	2.71
DB/U	NO_x Emission	87	291	90	Weibull	324	3.84
DB/LNB	Heat Rate	98	10,570	800	Lognormal	9.26	0.0774
DB/LNB	Capacity Factor	98	0.69	0.14	Beta	7.02	3.18
DB/LNB	NO_x Emission	98	176	42	Gamma	17.2	10.2
T/U	Heat Rate	136	10,860	1,340	Lognormal	9.28	0.113
T/U	Capacity Factor	136	0.62	0.15	Beta	6.08	3.79
T/U	NO_x Emission	136	196	55	Gamma	5.24	0.27
T/LNC1	Heat Rate	41	10,600	850	Normal	10,600	848
T/LNC1	Capacity Factor	41	0.69	0.14	Beta	6.53	2.94
T/LNC1	NO_x Emission	41	163	37	Gamma	19.0	8.58
DTF/OFA	Heat Rate	6	10,420	910	Lognormal	9.24	0.058
DTF/OFA	Capacity Factor	6	0.71	0.09	Beta	0.711	0.087
DTF/OFA	NO_x Emission	6	191	19	Gamma	99.5	1.91

* 1st parameter is the mean for Normal distribution, the geometric mean for the Lognormal distribution, scale parameter for he Gamma and the Beta distribution, and the shape parameter for the Weibull distribution.

* 2nd parameter is the standard deviation for the Normal distribution, the geometric standard deviation for the Lognomal distribution, and the shape parameter for Weibull, Gamma and Beta distributions.

The 50 percent confidence interval for the beta distribution fitted to the capacity factor data encloses 61 percent of the data, and 100 percent of the data are enclosed by the 95 percent confidence interval. Similarly, for the gamma distribution fit to the emission factor data, 57 percent of the data are enclosed by the 50 percent confidence interval and 100 percent of the data are enclosed by the 95 percent confidence interval. These comparisons indicate a good fit in either case.

Figures 2 through 4 reveal substantial inter-unit variability in emissions for the example technology group. The range of heat rate variability is from 9,100 BTU/kWh to 13,600 BTU/kWh. The capacity factor varies from 0.30 to slightly over 0.98. The emission factor varies from 80 g/GJ to 300 g/GJ. Thus, in some cases, the range of variability is almost a factor of four from the low to high end of the range.

In the example inventory, there are only 3 units of the specific technology group represented in Figures 2, 3, and 4. Thus, although there are a total of 98 such units represented in the database, the uncertainty estimate specific to the example inventory must account for the fact that there are only 3 units in the inventory. An assumption is that the 3 units are a random sample of the population of all units of the same technology group. Therefore, the uncertainty in the mean emission rate among the 3 units should be based upon a sample size of 3 and not a sample size of 98. Bootstrap simulation with bootstrap samples of 3 synthetic data points was used to quantify uncertainty.

An example of results for uncertainty based upon the number of units actually in the inventory is shown in Figure 5 for the case of the NO_x emission rate. In comparing Figure 5 with Figure 4, it is apparent that the confidence intervals are much wider, corresponding to the smaller sample size. With a smaller number of units, the range of uncertainty is larger.

Figure 2. Probability Band for Distribution Fitted to Example Heat Rate Data for Dry Bottom Wall-fired Boilers Using Low NO_x Burners (n=98)

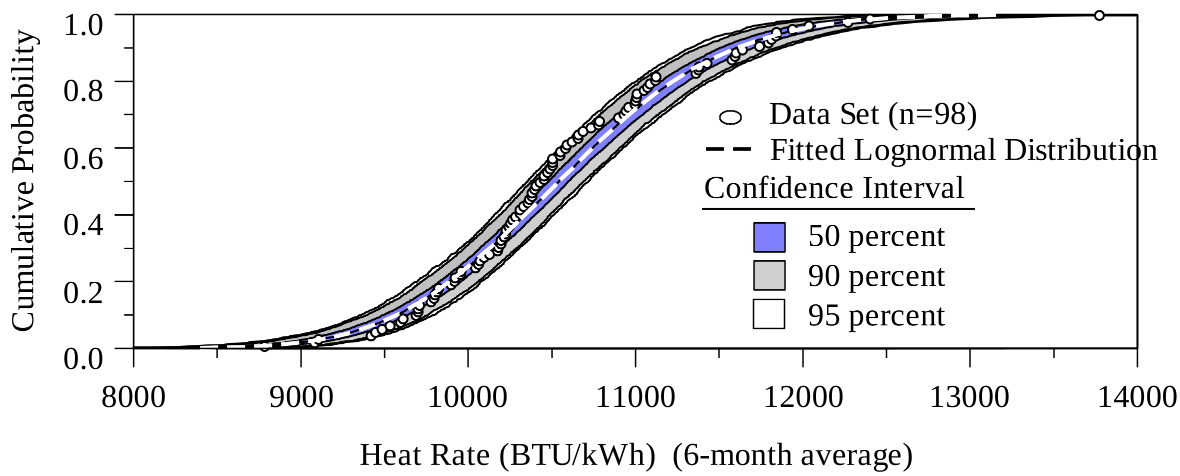


Figure 3. Probability Band for Distribution Fitted to Example Capacity Factor Data for Dry Bottom Wall-fired Boilers Using Low NO_x Burners (n=98)

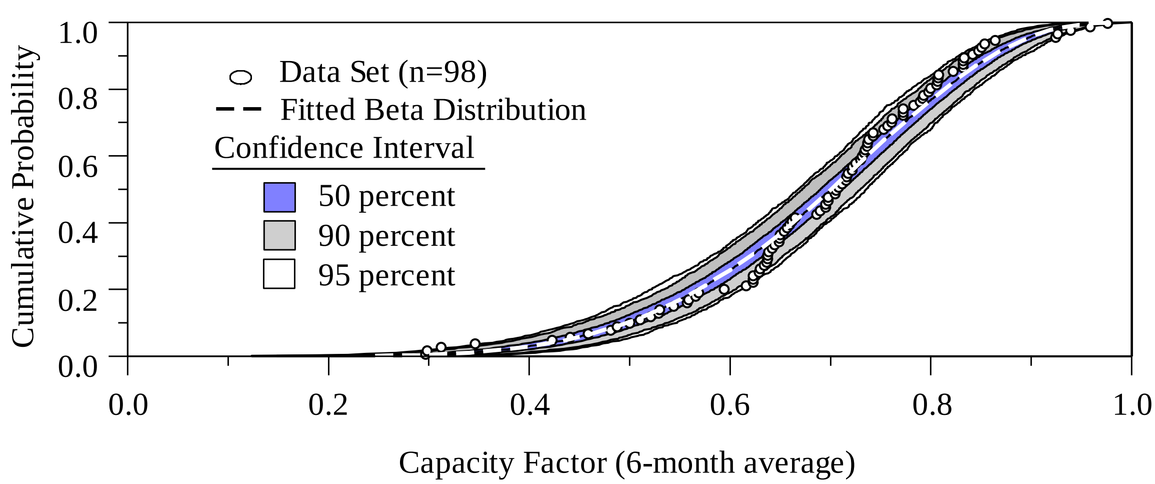


Figure 4. Probability Band for Distribution Fitted to Example NO_x Emission Rate Data for Dry Bottom Wall-fired Boilers Using Low NO_x Burners (n=98)

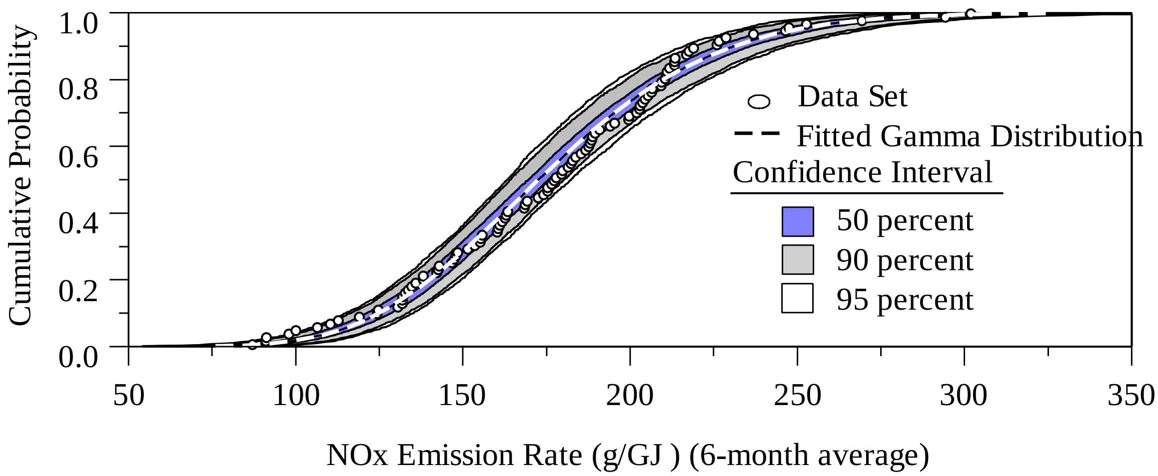


Figure 5. Probability Bands Based Upon Number of Units in the Emission Inventory (n=3) for the Example of NO_x Emission Rate.

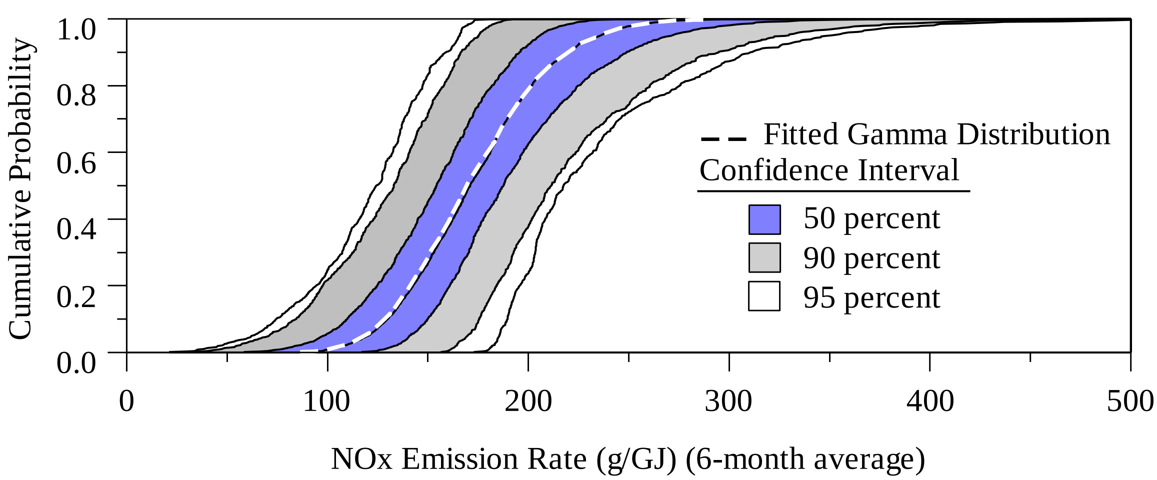


Table 2. Summary of Uncertainty Results for the Emission Inventory Case Study

Technology Group	2.5th Percent	Mean	97.5th Percentile	Random Error (%)[a]	
				Negative	Positive
DB/U	21,700	31,100	40,100	-30	+29
DB/LNB	5,600	8,100	11,400	-31	+39
T/U	15,300	20,400	28,600	-25	+40
T/LNC1	19,800	25,200	31,100	-21	+23
Total	71,800	84,800	99,900	-15	+18

[a] Results shown are the relative uncertainty ranges for a 95 percent probability range, given with respect to the mean value.

Figure 6 shows the sampling distribution of the mean emission inventory for the selected technology group. In this case, the emissions are from 3 units. The mean value of the inventory is 8,100 tons of NO_x emitted over a 6-month period. The 95 percent probability range for this distribution is from 5,600 tons to 11,400 tons, or almost a factor of two range of uncertainty. Expressed on a relative basis, the 95 percent probability range for uncertainty is minus 31 percent to plus 39 percent with respect to the mean value. The range of uncertainty is slightly asymmetric, reflecting the fact that many of the inputs have skewed distributions. The range of uncertainty reflects the large amount of inter-unit variability in the inputs to the inventory and the small sample size (n=3).

The overall uncertainty in the total emission inventory, inclusive of all four technology groups considered, is shown in Figure 7. The estimated mean emission rate is 84,800 tons of NO_x emitted in a 6-month period. The 95 percent probability range is enclosed by emissions of 71,800 tons and 99,900 tons. This is a range of – 13,000 tons to + 15,100 tons, or -15 percent to +18 percent, with respect to the mean. The asymmetry of the 95 percent probability range is a result of skewness in many of the input assumptions among the four technology groups.

A summary of the uncertainty results for the entire emission inventory is given in Table 2. The absolute range of uncertainty for the total inventory is greater than the absolute range of uncertainty for the selected technology group, but the relative range of uncertainty is smaller.

Figure 6. Uncertainty in a 6-Month NO_x Emission Inventory for an Individual Technology Group Comprised of 3 Units.

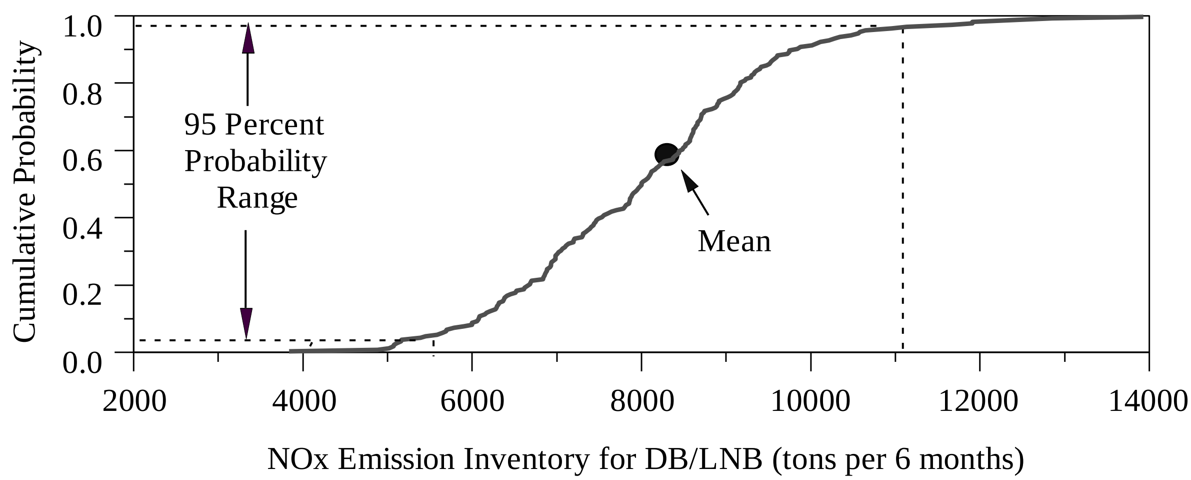


Figure 7. Uncertainty in a 12-Month NO_x Emission Inventory Inclusive of Four Technology Groups.

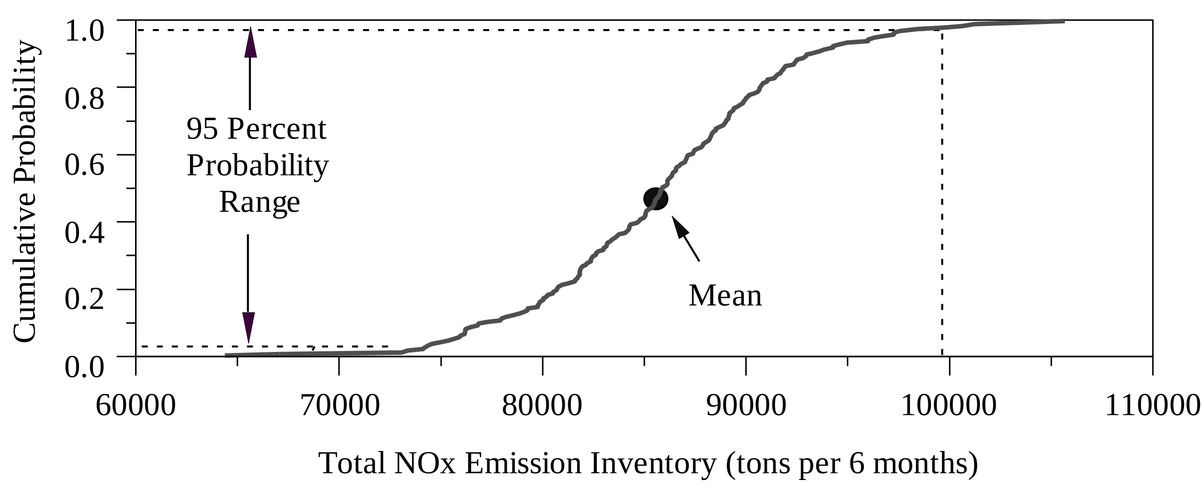
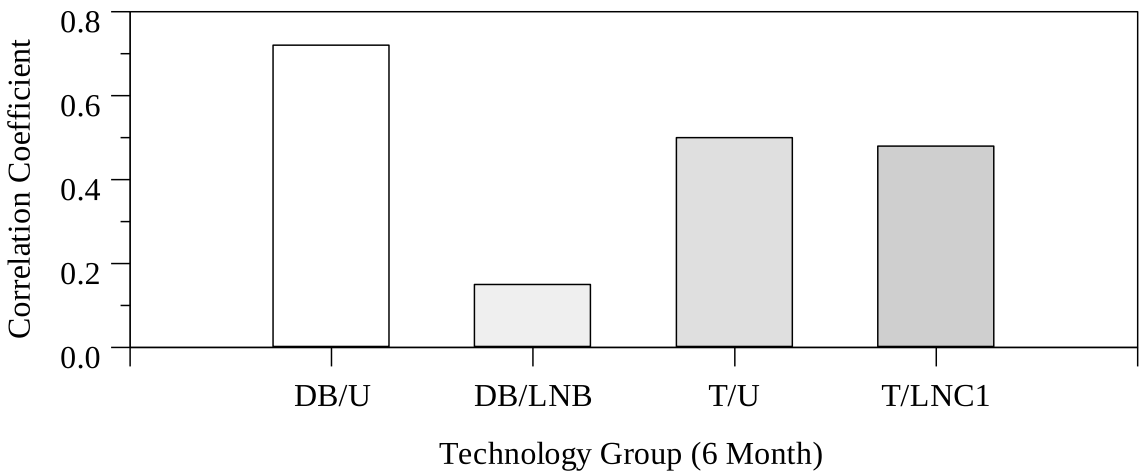


Figure 8. Relative Importance of Uncertainty in Emissions from Individual Technology Groups with Respect to Overall Uncertainty in the Total Emission Inventory



A property of probabilistic simulations is that, in general, it is not possible to sum the values of selected percentiles of each model input to obtain an estimate of the same percentile of the model output. For example, the 2.5th percentile of the total emission inventory, which is 71,800 tons, does not correspond to a sum of the 2.5th percentile of each of the four technology groups. However, for linear models, the sum of the means is usually the same as the mean of the sum, unless there is a correlation among the model inputs.[17]

Figure 8 shows the relative importance of uncertainty in emissions from individual technology groups with respect to overall uncertainty in the total emission inventory. Of the four technology groups, the dry-bottom, uncontrolled (DB/U) group has the strongest correlation with uncertainty in the total emission inventory, with a correlation coefficient of approximately 0.7. In contrast, the controlled dry-bottom boiler group (DB/LNB) has a correlation of approximately 0.18. Thus, any imperfections in the fitted distributions for the latter technology group are not likely to contribute significantly to errors in the estimated overall uncertainty. The sensitivity analysis results imply that the most effective way to reduce uncertainty in the overall emission inventory is to begin by reducing uncertainty in the estimated emissions from DB/U technology group.

CONCLUSIONS

This project has demonstrated a prototype software environment for calculation of probabilistic emission inventories. The prototype enables a user to visualize, in the form of empirical probability distributions, the data used to develop the inventory. Therefore, the user is able to observe the range of variability in the data. This is sharp contrast from typical emission inventory work, in which point estimate values of emission factors are used to calculate a single estimate of the inventory. The range of variability in the example datasets was shown to be large. For example, the range of inter-unit variability in emission factors for one technology group was a factor of approximately three from the smallest to the largest value in the dataset.

Although it is not possible to quantify all sources of uncertainty, it is important to quantify as many sources of uncertainty as is practical. The example case study demonstrates that the range of uncertainty attributable to random sampling error is substantial. For individual technology groups, the range of uncertainty is as large as approximately plus or minus 30 percent, and for the total inventory the range of uncertainty is approximately plus or minus 15 percent. These ranges of uncertainty are likely to be substantially larger than measurement errors in the data for this particular source category. The case study is based upon a relatively large sample of continuous emission monitoring data. Therefore, it is likely that the data used in the case study are reasonably representative of actual emissions among the population of units for the technology groups studied. In this case, it is likely that random sampling error is the most important contributor to overall uncertainty. The specific results will differ for other emission source categories.

It is now possible to have a high degree of uncertainty regarding recent actual emissions at power plants equipped with CEM equipment. However, it is not possible to have certainty regarding what the emissions will be at a future time, whether in the near or distant future. In estimating distant future emissions, an additional refinement that may be needed in the case study would be to consider changes in capacity factor and the effects of capacity expansion. For relatively short term future estimates (e.g., a year or two into the future), the methodology employed as is may provide a reasonable estimate of absolute emissions. However, the relative range of uncertainty estimated using the methods presented here are likely to be indicative of the relative range of uncertainty in a future emission inventory, unless there is a large shift in the relative contributions of different technology groups to the total inventory.

As part of future work, it is recommended that possibility for correlation in the distribution of uncertainties in mean capacity factors among different units be studied in more detail. Although such correlation is not expected to be significant for 6-month or 12-month averages, it will be useful to verify whether this is the case.

In addition to quantifying the substantial range of uncertainty in the inventory, the case study demonstrates the capability to identify key sources of uncertainty in the inventory. The largest contribution to uncertainty comes from one technology group. Therefore, resources could be focused on collecting more or better data for the most sensitive technology group. Knowledge of key sources of uncertainty can also aid in identifying where it is not necessary to target additional data collection. For example, even though there were some discrepancies in the fit of parametric distributions to some of the data as shown in Figure 2 that particular technology group does not contribute substantially to uncertainty in the overall inventory. Therefore, there would not be a large benefit associated with improving the characterization of uncertainty for that particular input.

The quantification of uncertainty has many important implications for decisions. For example, it enables analysts and decision makers to evaluate whether time series trends are statistically significant or not. It enables decision makers to determine the likelihood that an emissions budget will be met. Inventory uncertainties can be used as input to air quality models to estimate uncertainty in predicted ambient concentrations, which in turn can be compared to ambient air quality standards to determine the likelihood that a particular control strategy will be effective in meeting the standards. In addition, using probabilistic methods, it is possible to compare the uncertainty reduction benefits of alternative emission inventory development methods, such as those based upon generic versus more site-specific data. Thus, the methods presented here allow decision makers to assess the quality of their decisions and to decide on whether and how to reduce the uncertainties that most significantly affect those decisions.

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