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Quantification of Variability and Uncertainty in Emission Factors and Inventories

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Abstract

We demonstrate a quantitative approach to characterizing variability and uncertainty in emission factors, activity data, and inventories. The approach is illustrated for the case of NO_x emissions from selected types of coal-fired power plants. Variability refers to differences over time and/or location, whereas uncertainty arises because of lack of perfect knowledge regarding the true value of a quantity (e.g., emission rate) at a given place or time. We quantified variability in NO_x emissions for uncontrolled and controlled tangential-fired and dry bottom wall-fired boilers. Variability was quantified for 3 month and 6 month averaging times based upon Continuous Emission Monitoring System (CEMS) data reported to the U.S. Environmental Protection Agency. Uncertainty due to statistical sampling error was quantified using a numerical method known as bootstrap simulation. The sensitivity of uncertainty estimates to the number of plants included in an inventory was evaluated. Seasonal variability in 3 month average emissions was evaluated and not found to be significant, based upon currently available data. Emission factors, capacity factor, and heat rate data needed to develop an inventory were found to be approximately statistically independent. A partial probabilistic NO_x inventory was developed using utility data for North Carolina, to illustrate how uncertainties may be combined to estimate uncertainty in total emissions.

Introduction

Emission Inventories (EIs) are a vital component of environmental decision making. For example, emission inventories are used 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.

Emissions inventory work should include characterization and evaluation the quality of data used to develop the inventory. In this paper, we demonstrate a quantitative approach to the characterization of both variability and uncertainty as an important foundation for conveying the quality of estimates to analysts and decision makers. Variability is the heterogeneity of values with respect to time, space, or a population. Uncertainty arises due to lack of knowledge regarding the true value of a quantity. Variability in emissions arises from: variation in feedstock compositions; inter-plant variability in design, operation, and maintenance; and intra-plant variability in operation and maintenance. Uncertainty typically arises due 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. The method features the use of Monte Carlo and bootstrap simulation (Efron and Tibshirani, 1993; Frey, 1998a; Frey and Rhodes, 1998; Cullen and Frey, 1998), and has previously been demonstrated in the context of air toxics emissions estimation (e.g., Frey and Rhodes, 1996; Frey, 1998b). The method is illustrated by application to a case study regarding utility NO_x emissions. The example demonstrates how variability and uncertainty are a function of spatial (e.g., number of plants) and temporal (e.g., hourly, daily, monthly) averaging. The implications of the results for characterizing the quality of the inventory and for decision making are discussed.

The quantitative approach to probabilistic analysis of both variability and uncertainty employed in our work differs from the conventional approach to emission factor and inventory data quality ratings. Qualitative "A" through "E" ratings are defined and reported in EPA's Compilation of Air Pollutant Emission Factors (USEPA, 1995). The Data Attribute Rating System (DARS) is a method for combining data quality scores for both emission factor and activity data to develop an overall quality score for an emission inventory (Beck and Wilson, 1997). While DARS can enable comparison of quality ratings for emission inventories, it cannot be used to *quantify* the precision of an inventory, nor to evaluate the robustness of a decision to uncertainty. The probabilistic approach presented here enables quantification of the precision of an inventory, identification of key sources of uncertainty, and evaluation of the robustness of a decision to uncertainty (Frey, 1997; Frey and Rhodes 1996; Rhodes and Frey, 1997).

The qualitative emission factor rating methods differ from the quantitative approach described here in terms of input requirements. Nominally, the quantitative approach is based upon measured data, whereas the qualitative approaches are based upon expert judgment. However, both approaches require expert judgment. For example, expert judgment is required in the quantitative approach to decide which data are considered representative of the population of emission sources, whether the data are of sufficient quality, and what methods to use to analyze the data. Furthermore, it is possible to encode probability distributions based on formal protocols for expert elicitation (e.g., Morgan and Henrion, 1990). In this paper, we focus on quantitative analysis of data, rather than expert elicitation, as a basis for specifying probability distributions.

EXAMPLE CASE STUDY: UTILITY NO_x EMISSIONS

The probabilistic method for quantification of variability and uncertainty is demonstrated via a case study of utility NO_x emissions from coal-fired power plants. The example presented here is for a partial six-month inventory for the state of North Carolina. The inventory is partial because it includes only four power plant technologies, for which illustrative analyses of variability and uncertainty have been completed at this time. However, the approach can be extended to include all power plant technologies that would comprise the utility inventory of any given state.

The probabilistic analysis has focused upon characterization of variability and uncertainty in both activity and emission factor data. Power plant activity data which was characterized probabilistically includes individual unit heat rate (BTU of fuel input required to produce one kWh of electricity) and capacity factor (average capacity utilization for a specified time period). Capacities (MW) for individual units were assumed to be fixed quantities without uncertainty or variability. However, the approach could be extended to treat these quantities probabilistically if there was reason to believe that the reported capacities were in error, if the true maximum possible plant capacity had not yet been achieved in actual operation, or if the true capacity were to vary over time as the result of maintenance, repair, and upgrade/decommissioning procedures for the units in question. Compared to variability and uncertainty in heat rate and capacity factor, it is unlikely that uncertainty or variability regarding true plant capacity would play a significant role in most cases, other than due to data recording errors.

Data Used for Case Studies

The data used to develop probability distributions for heat rate, capacity factor, and emission factor were obtained from the Acid Rain Division of USEPA. There are three types of Summary Emissions Reports available via the World Wide Web. The reports used for this study are the ones which report quarterly values for the summary emissions for electric utilities regulated by the Acid Rain Program. Data from all four quarters of 1997 and the first quarter of 1998 are considered in this study, since these were the data available at the time that this project was initiated.

Each of the reports lists data at the stack and/or unit level depending on how the data are monitored and reported by the utility. All reports are organized in an alphabetically. The first level of organization is by state; within each state the reports are sorted by electric utility or holding company (with utility code in parentheses); within each utility or holding company is the name of the plant(s) owned or operated by that utility (with a U.S. Department of Energy plant code labeled "ORISPL" in parentheses). Finally, the data for each unit within the plant are shown.

The data for each quarter are stored in separate files. The descriptions for the fields of the tables containing the quarterly values used in this study are as follows:

- Unit/Stack ID: The name or number of the boiler or smokestack to which the data apply. The Unit/Stack ID coupled with the ORISPL can be used to uniquely identify each unit in the database.
- Boiler Type: The boiler technologies considered in this study are: (1) Dry bottom wall-fired (DB); and (2) Tangential-fired (T)
- Primary Fuel: The primary fuel considered in this study is coal (C) only.
- NO_X Controls: The types of operating pollution control devices at the units selected include: (1) Uncontrolled (U); (2) Low NO_X burner and overfire air option 1 (LNC1); (3) Low NO_X burners with Overfire air (LNBO). There are additional types of control technologies in the database which are not included in this study at this time.
- Total Operating Time: The number of hours the unit or stacks were operated during the quarter.
- Quarterly Gross Unit Load: The amount of electrical generation by each unit in megawatt-hours.
- Total Quarterly Heat Input: The caloric value of the fuel burned at the unit during the quarter, in millions of British thermal units (BTU).
- Average Hourly NO_X Emission Rate: The average of NO_X emitted to fuel burned during the quarter, reported in pounds of NO_X (as NO_2) per million BTU.

The above database was merged with another database supplied by USEPA which contained the values of the reported maximum megawatt load for each of the units in the above database. The maximum megawatt load was used as a measure of the plant capacity for the purpose of calculating an average capacity utilization factor. The heat rate and capacity factor values used in this study were calculated from the data obtained in the merged database.

Description of Technologies

Four coal-based power generation technologies were selected for this study. These included dry bottom wall-fired boilers and tangential-fired boilers, each with and without combustion-based NO_x controls.

The state of North Carolina was selected as a basis for an illustrative case study because the number of units representing each of the four technologies are dissimilar. Thus, there would be different amounts of uncertainty, based on random sampling error, associated with the emissions estimates for each of the four technologies. Specifically, the following numbers of units are included in the partial emission inventory:

- 26 tangential-fired boilers with no controls
- 12 tangential-fired boilers with controls
- 8 dry bottom wall-fired boilers with no controls
- 3 dry bottom wall-fired boilers with controls

The disparate number of units, representing each of the four technologies mentioned above, presents a unique opportunity for understanding the role of averaging over different numbers of units with respect to uncertainty in emissions for technology groups and statewide emissions from all four technologies.

METHODOLOGICAL APPROACH

The general approach employed to quantify variability and uncertainty in an emission inventory includes the following major steps:

1. Assemble and evaluate a database
2. Visualize data by developing empirical cumulative distribution functions for individual variables and scatter plots to evaluate dependencies among pairs of variables
3. Select, fit, and critique alternative parametric probability distribution models for representing variability in activity and emissions factors
4. Characterize uncertainty in the distributions for variability
5. Evaluate the effect of averaging, over both time and space, on variability and uncertainty
6. Propagate uncertainty and variability in activity and emissions factors to estimate uncertainty in statewide emissions.

The first step, assemble and evaluate a database, was described in the previous section. The remaining steps are illustrated with examples.

Variability and Uncertainty in Emission Inventory Inputs

As an example of variability in activity data needed for an emission inventory, we consider the capacity factor for dry bottom wall-fired boilers with low NO_x burners and overfire air, as shown in Figure 1. Since our objective for the illustrative emission inventory was to focus on the months associated with the ozone season, we combined second and third quarter data from 1997 to create estimates of the six-month average capacity factor for each of eight units in the database of the selected technology type. The six-month average capacity factor varies from approximately 0.4 to 0.8 among the eight units.

Because capacity factor must be bounded by zero and one, we selected a Beta distribution as a probability distribution model appropriate for representing an estimated population distribution of capacity factors for the selected technology. We used the maximum likelihood estimation method to estimate the parameters of the Beta distribution from the eight data points. The fitted distribution is shown as a dashed line in Figure 1. The fit, although not perfect, appears to be reasonable; all of the data points are reasonably close to the fitted distribution.

However, in order to evaluate the adequacy of the fit, and to characterize uncertainty in the estimated population distribution, we performed bootstrap simulation. Bootstrap simulation, described in detail by Efron and Tibshirani (1993), is a numerical technique originally developed for the purpose of estimating confidence intervals for statistics. This method has an advantage over analytical methods in that it can provide solutions for confidence intervals in situations where exact analytical solutions may be unavailable and in which approximate analytical solutions are inadequate.

The approach in bootstrap simulation is conceptually straightforward. An assumed population distribution is developed, such as by fitting a parametric distribution to a dataset. Then, a simulated random sample of data points of the same sample size as the original data is drawn from the assumed distribution. This simulated data set may be referred to as a "bootstrap sample." The statistic(s) of interest are calculated for the bootstrap sample. For example, if we are interested in knowing the confidence interval for the mean, we would calculate the mean value of the bootstrap sample. The estimate of a statistic for a bootstrap sample is referred to as a "bootstrap replication" of the statistic. This process is then repeated many times (perhaps 500 to 2000 times) to create a probability distribution of bootstrap replications of the statistic. A probability distribution for a statistic is also referred to as a "sampling distribution." From the sampling distribution, confidence intervals can be inferred. For example, a 95 percent confidence interval would be enclosed by the 2.5th and 97.5th percentiles of the sampling distribution.

In the example of Figure 1, confidence intervals are calculated for many percentiles of the fitted probability distribution. This was done by fitting a probability distribution to each bootstrap replication, and then determining the value of the fitted distribution associated with selected percentiles. By repeating this process, a sampling distribution for each percentile was developed. The 50, 90, and 95 percent confidence intervals for each percentile were then estimated. For example, the 95 percent confidence interval for the 20th percentile is enclosed by capacity factors of 0.33 and 0.55. The 95 percent confidence interval for the median (50th percentile) is enclosed by values of 0.45 and 0.65. If we interpret these confidence intervals as uncertainty, then we could refer to the 95 percent confidence interval as being a 95 percent probability range.

An important insight obtained from bootstrap simulation is the adequacy of a fitted probability distribution model. The results in Figure 1 indicate that approximately half of the data points are enclosed by the 50 percent confidence interval for the fitted distribution, and all of the data points are within the 90 percent confidence interval. Thus, the fitted distribution appears to be an adequate description of the data.

A similar case study is given in Figure 2 for variability and uncertainty in the NO_x emission factor on a fuel input basis. After evaluating several alternative probability distribution models, including lognormal and Weibull distributions, a Gamma distribution was selected as the most adequate fit to the eight data points. The fitted distribution represents an estimate of the variability in six-month average emissions for this type of technology. The distribution implies that 95 percent of these types of plants would have an emission rate between approximately 120 g/GJ and 350 g/GJ. The confidence intervals on the fitted distribution were developed using bootstrap simulation in the same manner as for the capacity factor example. The width of the 95 percent confidence interval is approximately a span of 100 g/GJ at the median value, indicating that the nominal uncertainty range is of the same order of magnitude as the observed range of variability in emissions. Hence, both uncertainty and variability should be considered.

Effect of Averaging on Variability and Uncertainty Estimates

Emissions inventories are developed for a variety of averaging times and geographic areas. Here, we illustrate how averaging over both time and space impacts the estimate of variability and uncertainty in emissions. For example, in Figure 3, there is a comparison of the distribution of variability for a three-month versus a six-month average emission rate. Although somewhat difficult to see clearly in this example, it is the case that as averaging is done over longer time intervals, there is less variability. Similarly, Figure 4 indicates that mean emissions estimated for larger populations of plants have narrower ranges of uncertainty than mean emissions estimated for smaller populations. For example, the 95 percent probability range for mean emission rate for five units ranges from approximately 145 g/GJ to 195 g/GJ, whereas the corresponding uncertainty range for 20 units is much narrower, ranging from approximately 160 g/GJ to 175 g/GJ.

Seasonal Variability and Emissions

We searched for possible seasonal trends in activity or emission factors with the available data. Figure 5 is an example in which the mean and standard deviation of quarterly distributions for emission factors were compared for one type of technology. Also shown are the 95 percent confidence intervals for both the mean and standard deviation. Each point and set of confidence intervals represents one season. The standard deviations and confidence intervals for standard deviations for all four seasons are nearly identical, indicating similar ranges of variability in emissions for the four seasons. The mean values are not statistically different from each other. Therefore, in this case, we conclude that the emission factor is invariant with respect to season.

Dependencies Between Variables

To evaluate possible dependencies among variables, we calculated correlation coefficients and also developed scatter plots of the data for one emission inventory input versus another input. For example, Figure 6 shows the emission factor plotted versus the capacity factor for one technology data set, both based on six month averages. The graph indicates that the range of variation in the emission factor is approximately the same regardless of the average capacity factor, and the emission factor shows no systematic trend as capacity factor changes. Therefore, we conclude in this case that the variation in emission factor can be treated as statistically independent of the variation in capacity factor. Of course, this conclusion may not hold in general for other data sets.

Examples of Probabilistic Emission Inventories

To illustrate the process of calculating probabilistic emission inventories, we present an example summarized in Figures 7, 8, and 9. Figure 7 is a table illustrating a point-estimate approach to developing an inventory. The point estimates used are based upon average values for each of the four types of technologies considered. The averages were calculated from all data reported in the EPA database, which includes power plants in many states. Heat rate, capacity factor, and emission factor data were obtained in this manner. The total plant capacity data were obtained from the EPA database for the selected technologies for the state of North Carolina, for the purpose of illustrating the development of a state inventory. The total emissions for each of the four technologies were calculated and then summed to yield a partial total utility emission inventory. The purpose of this inventory is not to be a complete representation of all emissions in the state. Rather, it is to serve as a point of comparison with the probabilistic results.

The probabilistic inventory was simulated by using the fitted probability distributions for each of the three input variables (heat rate, capacity factor, and emission factor) obtained from analysis of six month average estimates for four technologies based upon the EPA database. A probabilistic modeling framework based upon that used by Frey and Rhodes (1998) was employed. In this framework, bootstrap simulation was used to estimate uncertainty ranges for each fitted distribution for the inventory inputs. The uncertainty was estimated based upon the number of power plants of each type in the state of North Carolina. For example, since there are 26 uncontrolled tangential fired boilers with no controls listed in the EPA database for the state of North Carolina, 26 samples were drawn at random from the heat rate distribution that was fitted to the data for all such boilers in all states. The assumption here is that units in North Carolina are not fundamentally different in design or operation than those in other states. Each of the 26 samples was assigned to an individual unit with a known plant size. Simultaneously, 26 values were sampled from the fitted distributions for capacity factor and emission factor. Thus, for each of the 26 units in the state, synthetically sampled values were used for heat rate, capacity factor, and emission factor, with the known value of unit capacity, to estimate a unit-specific total emission. The emissions were summed across all 26 units to develop a technology-specific total. This process was repeated many times, with different sets of random samples, to come up with alternative possible emission inventories. Hence, a distribution was developed for the uncertainty in the emissions for each individual unit, as well as for the total of all units within a technology. This process was conducted for all four technology groups.

The overall uncertainty in the emission inventory is shown in Figure 8. The point estimate from the table in Figure 7 is 79,000 tons over the six-month period. The estimate of uncertainty in this total has a 95 percent probability range from approximately 60,000 tons to approximately 100,000 tons, or approximately plus or minus 25 percent of the nominal value. However, the distribution for uncertainty in the total is not exactly symmetric with respect to the point estimate. It appears in this case that there is approximately a 60 percent probability that the emissions may be lower than the point estimate.

It is possible to apportion the total emissions among the four technologies, as shown in Figure 9. These results indicate that the largest contribution to total emissions may be from either uncontrolled dry bottom wall-fired boilers or uncontrolled tangential-fired boilers. Since the uncertainty distributions for these two overlap, it is ambiguous as to which of these two technologies may have the largest share of total emissions. However, it appears likely the tangential-fired units, of which there are 26, are the major contributor. In contrast, as expected, the controlled technologies contribute a relatively small portion of the total emissions. Even when uncertainty is considered, it is clear, for example, that controlled dry bottom units as a group contribute less than uncontrolled dry bottom units.

Using similar types of analyses, it would be possible to compare emissions from different source categories or different geographic regions to determine which ones contribute the most or least to an inventory, and to identify whether there is uncertainty regarding what the largest sources of emissions are. If there was a need to reduce uncertainty in an inventory, this type of information is useful in helping to pinpoint those source categories or regions for which more data would be helpful.

DISCUSSION

In this paper, we have presented by example an approach for quantifying variability and uncertainty in the inputs to an emission inventory, and for estimating the uncertainty in an emission inventory. We have used the example of utility NO_x emissions based upon data available from USEPA. We developed databases for both activity factors and emission factors needed to calculate a utility emission inventory. For those inputs which vary among different units within a source category, we developed probability distributions for variability using standard statistical techniques. In addition, we used the numerical method of bootstrap simulation to estimate the uncertainty in the fitted distributions. The "two-dimensional" probability distributions were used as inputs to a probabilistic simulation of a partial state-wide emission inventory for a summer ozone season. The distributions of variability in activity and emissions factors were used to sample and assign random values to each of the units within a state in order to come up with one possible inventory. The process was repeated with alternative random samples from the fitted distributions for the activity and emission factors to produce alternative possible emission inventories. These alternative inventories were then used to describe a probability distribution for uncertainty in the inventory. For the example case study, the uncertainty was approximately plus or minus 25 percent of the nominal point estimate value, for a 95 percent probability range. This range of uncertainty appears to a reasonable representation of the level of precision that can be expected in an inventory that is developed using generic data for a well-characterized source category and pollutant such as power plants and NO_x. However, it should be expected that the range of uncertainty in an inventory will differ for different source categories and pollutants.

CONCLUSIONS

The project has demonstrated a probabilistic approach for development of emission inventories. Because of the widespread use of inventories for policy making, planning, and research purposes, it is important that the quality of the inventories be known and that any shortcomings in the inventories be identified and prioritized for improvement. The method illustrated here enables quantification of the precision of the inventory, identification of key emission sources in the face of uncertainty, and identification of key sources of uncertainty that can be targeted for reduction via additional data collection and research. The latter is especially a critical concern when allocating scarce dollars to potentially expensive field studies or surveys.

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.

Figure 1. Comparison of Fitted Distribution for Variability in Six-Month Average Capacity Factor, with Bootstrap Confidence Intervals, to Data for Dry Bottom Wall-fired Boilers with Low NO_X Burners Having Overfire Air.

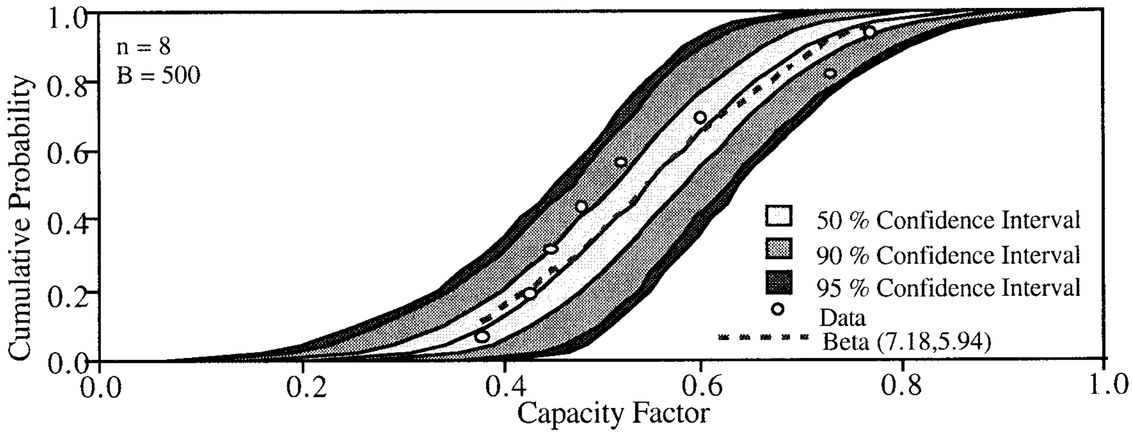


Figure 2. Comparison of Fitted Distribution for Variability in Six-Month Average Emission Factor, with Bootstrap Confidence Intervals, to Data for Dry Bottom Wall-fired Boilers with Low NO_X Burners Having Overfire Air.

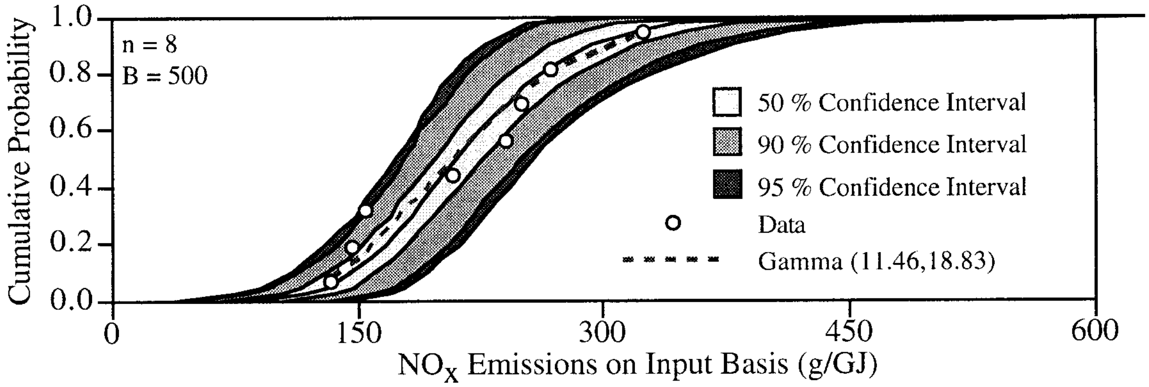


Figure 3. Comparison of 3-month and 6-month Variability in NO_X Emission Factor (g NO_2/GJ fuel input) for Tangential-fired Boiler with Low NO_X Coal and Overfire Air. Number of Data Points: 3-month = 198, 6-month = 26

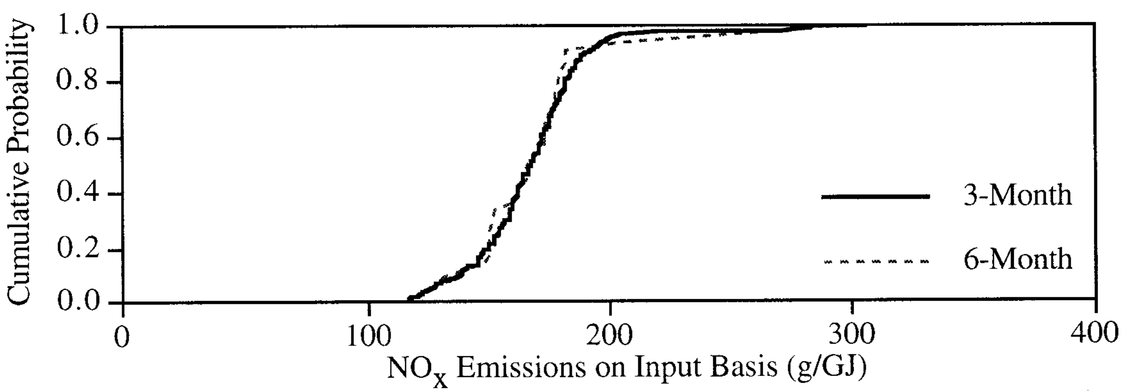


Figure 4. Uncertainty in Mean NO_X Emission Factor (g NO_2/GJ of fuel input) for Tangential-fired Boiler with Low NO_X Coal and Overfire Air Option 1 (6-month average).

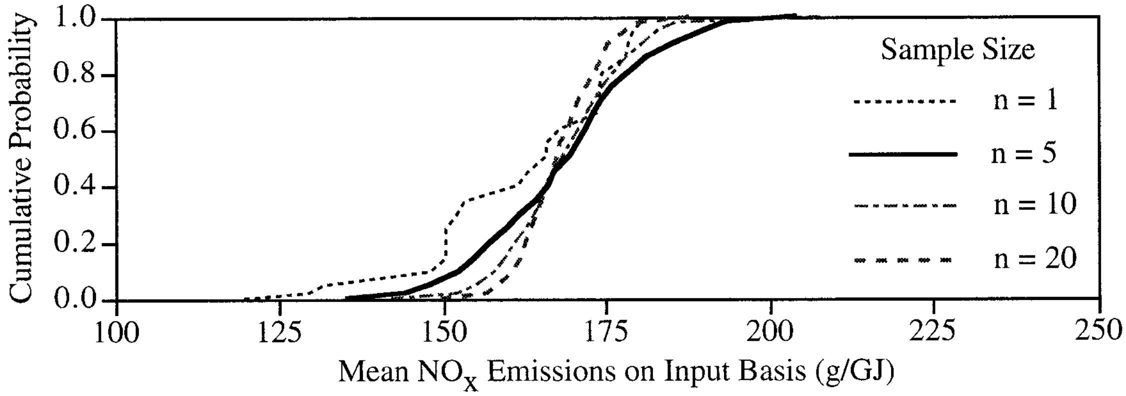


Figure 5. Mean Versus Standard Deviation with 95% Confidence Intervals, for Each of the 4 Seasons for NO_X Emission Factor (g NO_2/GJ of fuel input) for the year 1997 for Tangential-fired Boiler with Low NO_X Coal and Overfire Air.

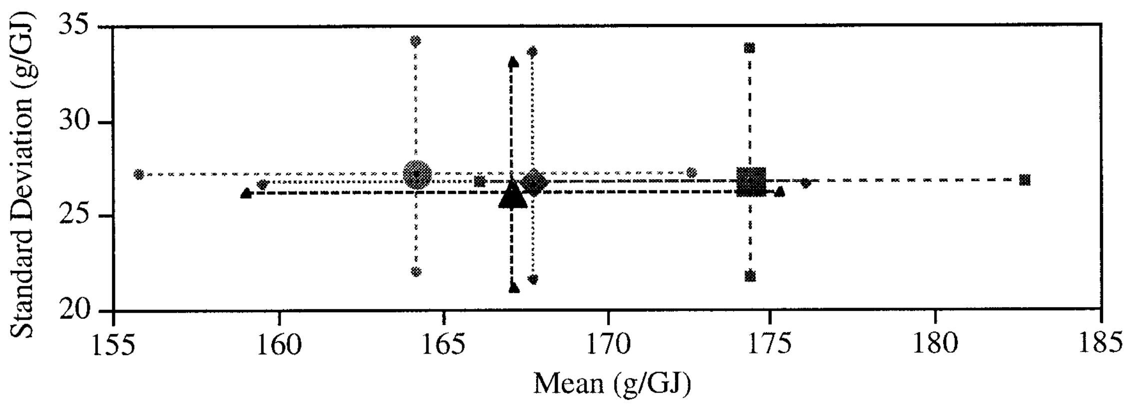


Figure 6. Scatter Plot of Six Month Average NO_X Emissions versus Six Month Average Capacity Factor for Low NO_X Coal and Overfire Air in Coal-Fired Tangential Boilers, Based on 2^{nd} and 3^{rd} Quarters of 1997.

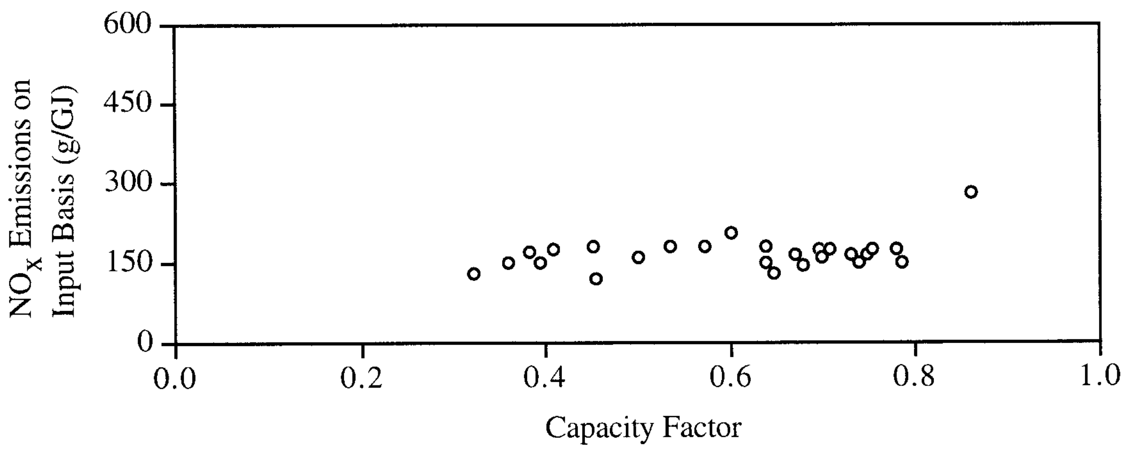


Figure 7. Summary of Example Partial Utility NO_x Six Month (Summer Season) Emission Inventory for North Carolina Using Mean Values of Activity and Emission Factor Data for Four Selected Technologies

Tech. Index	Boiler Type	NO_x Control	Mean Values: Heat Rate (Btu/kWh)	Capacity Factor	NO_x Emissions Input Basis (g/GJ)	Total Capacity (MW)	Total NO_x Emissions (Tons)
1	Dry Bottom	LNBO	10350.0	0.55	216	1,163	7,300
2	Dry Bottom	U	11250.0	0.51	315	3,013	27,700
3	Tangential	LNC1	10640.0	0.61	168	1,151	6,400
4	Tangential	U	11000.0	0.58	199	5,842	37,600
Totals						11,169	79,000

Figure 8. Uncertainty and Point Estimates for Partial Utility NO_X Emission Inventory for the State of North Carolina. (Based on Six-month Average Data)

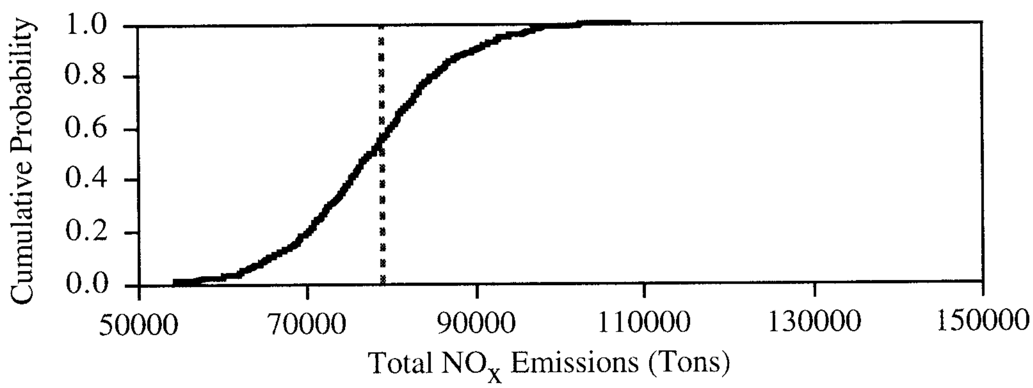
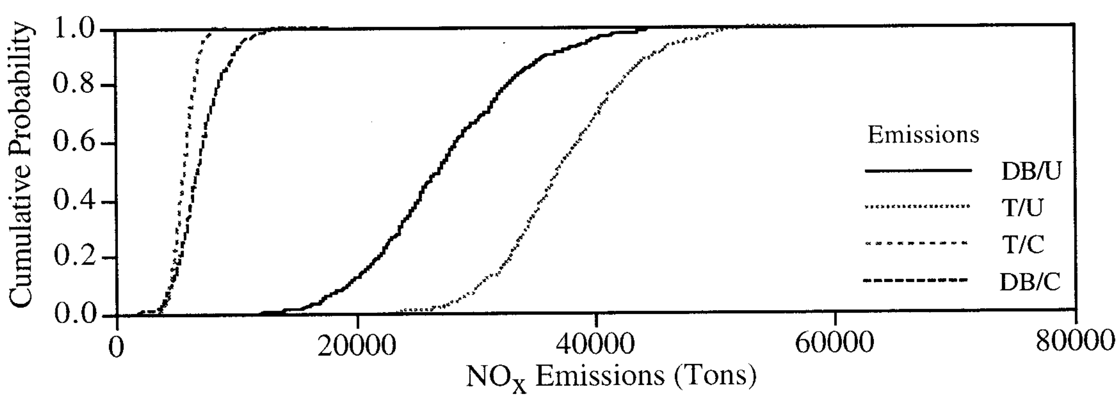


Figure 9. Uncertainty Estimates for Utility NO_X Emissions for Selected Technologies for North Carolina (Based on Six-month Average Data). Key: DB = Dry Bottom Wall-Fired Boiler; T = Tangential-fired; U = Uncontrolled; C = Controlled (e.g., Low NO_x Burners)



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