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Quantification of Variability and Uncertainty in Stationary Natural Gas-fueled Internal Combustion Engine NO_x and Total Organic Compounds Emission Factors

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H. Christopher Frey
Department of Civil Engineering, North Carolina State University, Raleigh, NC 27695

Song Li
Department of Civil Engineering, North Carolina State University, Raleigh, NC 27695

ABSTRACT

Quantitative methods for characterizing both variability and uncertainty are applied to case studies of emission factors for stationary natural gas-fueled internal combustion engines. NO_x and Total Organic Carbon (TOC) emission data sets for lean burn engines were analyzed. Data were available for uncontrolled engines and for engines with pre-combustion chamber (PCC) and "clean burn" NO_x control approaches. For each data set, parametric probability distributions were fit to the data using maximum likelihood estimation to represent inter-engine variability in emissions. Bootstrap simulation methods were used to quantify uncertainty in the fitted distribution and uncertainty in the mean emission factor. Some methodological challenges were encountered in analyzing the data. For example, in one instance, only five data points were available, with each data point representing a different market share. Therefore, an approach was developed in which a parametric distribution was fitted to population-weighted data. The range of uncertainty in mean emission factors ranges from approximately plus or minus 10 percent to as much as minus 60 percent to plus 80 percent, depending on the pollutant, control technology, and nature of the available data. The wide range of uncertainty in some emission factors emphasizes the importance of recognizing an accounting for uncertainty in emissions estimates. The skewness in some uncertainty estimates illustrates the importance of using a numerical simulation approach that does not impose restrictive symmetry assumptions on the confidence interval for the mean. In this paper, we briefly present the probabilistic analysis method, the data sets, the results of the analyses, and key findings and recommendations. Recommendations include reporting requirements for emission factor data.

1.0 INTRODUCTION

This paper focuses on demonstrating the use of quantitative methods for characterizing variability and uncertainty applied to emission factors. Emission factors are a key input to emission inventories. Emission inventories, in turn, are widely used for regulatory and air quality management purposes. However, the uncertainty in emission factors, and in emission inventories, is typically not known. Therefore, it is not known, in many cases, how robust regulatory or management decisions are with respect to uncertainty. For example, emission inventories are used to evaluate statewide compliance with emissions budgets, to assess emissions trends, for various regulatory analyses associated with permitting of new sources, to assess baseline and trends in air quality using air quality models, and for other applications. If unquantified errors or uncertainties exist in the emission factors and, hence, the emission inventories, then it is likely that the significance of trends, of comparisons of emissions before and after control strategies are implemented, and of air quality predictions using air quality models, are misestimated or not robust with respect to uncertainty. A regulatory or air quality management decision would be robust to uncertainty if the outcome of the decision led to net benefits even though the true value of emissions is not known precisely. In contrast, if management decisions are based upon point estimates of emissions that are biased, or if the range of uncertainty in emissions is much larger than any predicted change in emissions resulting from an air quality management strategy, then the decision-making process for developing management strategies will be ineffective. Because air quality management involves high stakes, such as public health, money, and other impacts, it is important that these decisions be based upon the best information available, and that they be robust to uncertainty. This paper focuses on one of the fundamental starting points for characterizing uncertainty in emission inventories, which is the emission factor. The case study application is stationary natural gas-fueled internal combustion engines.

1.1 Variability and Uncertainty

For a given emission source category, there is both variability and uncertainty in emissions. Emissions vary from one specific source to another (e.g., one engine to another) within a source category because of variations in design, feedstock compositions, ambient conditions, and other operating conditions. For a given specific source (e.g., a particular engine), emissions vary over time because of differences in feedstock composition, ambient conditions, other operating characteristics, and maintenance and repair. Thus, there is typically some inherent variation in emissions that is revealed by measurements on multiple specific emission sources or by repeated measurements of the same emission source.

For the purposes of developing emission factors, we are typically interested in knowing the average emission rate for a particular averaging time. For example, for purposes of developing an estimate of annual emissions, an annual average emission factor is needed. For purposes of developing hourly estimates of emissions for input to a photochemical air quality model, hourly average estimates of emissions would be needed. However, data are often not available to assess the variation in average emission factors for any arbitrary averaging time. Instead, data are often obtained based upon short term measurements that may not be directly relevant to the averaging time needed for an emission factor estimate.

Uncertainty refers to lack of knowledge regarding the true but unknown value of a quantity, such as the true but unknown population average emission factor for a particular source category. The average emission factor, even if for the correct averaging time needed for a particular type of analysis, is subject to uncertainty for several possible reasons: (1) random sampling error; (2) measurement errors; (3) non-representativeness of available data; and/or (4) lack of information. There is also the possibility that there are data entry mistakes. In this paper, the main focus is on quantification of random sampling error, which is the statistical random fluctuation in any statistic estimated from a finite random sample of data. Any statistic estimated from a random sample of data is itself a random variable. For example, the sample mean is a random variable. The probability distribution for a statistic is referred to as the sampling distribution. The sampling distribution can be used to develop confidence intervals for a statistic. In this paper, we use sampling distributions as a method for quantifying uncertainty associated with random sampling error.

1.2 Estimation of Uncertainty in Emission Factors

Current practice in emission inventory work is typically to ignore uncertainty. Uncertainties in emission factors and emission inventories are typically not reported. As a surrogate for uncertainty estimates, some emission factors are accompanied by data quality ratings, such as those reported in AP-42.[1] "A" to "E" qualitative ratings are assigned to emission factors as a indicator of their quality. A method for qualitatively rating emission inventories, known as the Data Attribute Rating System (DARS) has been developed by EPA.[2] Qualitative ratings of emission factors and emission inventories are important. Some sources of uncertainty are difficult to quantify, such as non-representativeness of a data set. Therefore, there will always be a role for qualitative statements regarding non-quantifiable sources of uncertainty. However, qualitative rating systems should be used in combination with quantitative approaches.

There is growing recognition of the importance of quantitative uncertainty analysis in environmental modeling and assessment. For example, the U.S. EPA has developed guidelines for Monte Carlo analysis of uncertainty.[3] The National Academy of Sciences has repeatedly recommended to EPA that quantitative analysis of uncertainty be included in a variety of applications.[4,5]

As part of previous and ongoing work, research is underway to develop and demonstrate improved methods for quantifying uncertainty in emission inventories. In the area of mobile source emissions, for example, Kini and Frey developed quantitative estimates of uncertainty associated with the Mobile5b emission factor model estimates of light duty gasoline vehicle base emissions and speed-corrected emissions.[6] Pollack *et al*. performed a similar study on California's EMFAC7G highway vehicle emission factor model.[7] Frey *et al*. revisited the earlier analysis of Mobile5b emission factor estimates to include uncertainties associated with temperature corrections.[8] Bammi and Frey estimated uncertainty in the emission factors for a non-road source category of lawn and garden equipment.[9] A recent National Research Council report has recommended that the U.S. Environmental Protection Agency (EPA) and others "should undertake the necessary measures to conduct quantitative uncertainty analyses of the mobile source emissions models."[4]

In the area of power plant emissions, Frey and colleagues have developed uncertainty estimates for emissions of hazardous air pollutants and for NO_x emitted by coal-fired power plants.[8,10,11,12] In addition, as part of recent work, methods for quantification of variability and uncertainty have been developed, evaluated, and demonstrated, including the use of Monte Carlo simulation and bootstrap simulation.[13,14,15]

In this paper, quantitative methods for characterizing variability and uncertainty are applied to the source category of stationary natural gas-fueled internal combustion engines. These engines are commonly used, for example, to power natural gas pipeline compressors. In some airsheds, such as for Charlotte, NC, this type of emission source is estimated to be a significant contributor to the total NO_x emission inventory.

2.0 OVERVIEW OF METHODS FOR PROBABILISTIC ANALYSIS OF EMISSION FACTORS

There are a variety of methods for quantification of uncertainty in environmental models, including analytical methods, approximate analytical methods, and numerical methods.[16] Analytical methods work only in a limited number of application areas, and often are not useful for many practical problems. Approximation methods, such as those based upon Taylor series expansions, have the potential for comparatively fast computation times but can suffer from inaccuracies or biases if models are highly nonlinear and/or if non-symmetric assumptions are made regarding probability distributions for model inputs. Numerical methods are typically more robust in that they can be applied to a wide range of problems without restrictive assumptions regarding probability distributions assigned to model inputs and for a wide variety of model formulations. Thus, in this work, numerical methods are employed.

The basic approach in probabilistic analysis is to quantify uncertainty in the inputs to a model, propagate the uncertainties through the model to make predictions of uncertainties in model outputs, and analyze the results. Using numerical methods, it is possible to specify dependencies among model inputs (if known) and to analyze simulation results to identify the key sources of uncertainty in model inputs contributing most to uncertainty in model outputs. There are a variety of specific simulation methods available. In this work, traditional Monte Carlo simulation is employed. The Monte Carlo approach was developed by Stanislaw Ulam and John von Neumann to simulate probabilistic events for military purposes in 1946.[17] Monte Carlo simulation is a numerical method for randomly generating sample values from a specified population distribution. The details of how the method works are reported elsewhere.[16]

This paper focuses on the characterization of variability and uncertainty in emission factors, which are inputs to emission inventories. Therefore, in this paper, we focus on methods for specifying probability distributions for a given model input. Methods for propagating uncertainty through models and for analyzing results are described elsewhere.[16]

2.1 Characterizing Variability in a Data Set

A first step in characterizing variability in a data set is to obtain all relevant data and assess the quality of the data. A judgment must be made that the data are a reasonably representative sample of the population of interest, and that the data are free of significant errors. This step is the same regardless of whether one is developing a point estimate or a probabilistic estimate. This is the most critical step in the analysis.

A second step is to visualize the data to obtain insight regarding the range, central tendency, and skewness of the data, and any other noteworthy characteristics. A method often employed for this purpose is to plot the data as an empirical cumulative distribution function (CDF). Methods for plotting empirical CDFs are described by Cullen and Frey and by Frey *et al*.[16,8]

It is convenient to represent a data set with a parametric probability distribution. While an empirical CDF is also a valid representation of a data set, the empirical CDF has some limitations. In particular, in a strict empirical CDF, each observed data point is assigned an equal probability, and no probability is assigned to any values other than those actually observed.

Therefore, there is no interpolation among the observed data, and there is no extrapolation beyond the range of observed data. The former is not a significant problem, but does tend to lead to "noisy" results when viewing the CDF of model outputs. The latter is a significant problem. Especially for small data sets, the range of sample observations for variability in emissions may be much narrower than the unknown true range of variability in the population. If additional data were to be collected, it is likely that some new observations would be less than the minimum value of the original sample, or greater than the maximum value of the original sample. Parametric probability distributions have an underlying theoretical basis. To the extent that the theoretical basis of the parametric distribution is based coincides in some way with the processes that lead to variation in the observed data, parametric distributions can provide a plausible means for extrapolating to the unobserved tails of the unknown population distribution. Parametric distributions also offer an advantage of compactness: an entire distribution can be represented by a specific formula for the distribution and by the numerical values of the parameters of the distribution. Most commonly used distributions have only two parameters.

The investigator's experience is very important in the selection of a parametric distribution. *A priori* knowledge of the theoretical basis for different distributions, and of the processes leading to variability in a data set, can aid in identifying candidate distributions for fitting to the data. For example, the normal distribution arises as a result of unbiased random processes, whereas Lognormal distributions often arise as a result of mixing or dilution processes. Theoretical considerations in the selection of distributions are discussed elsewhere.[16] In this study, Normal, Lognormal, Gamma, and Weibull distributions are considered.

After choosing a candidate parametric distribution, the next step is to estimate its parameters based upon the observed data. There are several methods for estimating distribution parameters, including, for example, probability plots, the method of matching moments, maximum likelihood estimation (MLE), and others. No method is necessarily the best one to use in all situations. However, MLE is considered to be a statistically efficient method and is reasonably robust.[16] Therefore, it is used in this work.

2.2 Characterizing Uncertainty

The previous section describes how variability in a data set may be represented by a parametric distribution. In this section, a method, based upon bootstrap simulation, for characterizing uncertainty in any statistic estimated based upon the parametric distribution is presented.[18]

The objective of bootstrap simulation is to numerically simulate sampling distributions for statistics. The main assumption in bootstrap simulation is that the probability distribution estimated from the observed sample of data is the best estimate of the true but unknown population distribution. Given the assumption of an assumed population distribution, the effects of random sampling from the population distribution are simulated. Specifically, a synthetic data set, known as a *bootstrap sample,* is sampled at random from the assumed population distribution using Monte Carlo simulation. The bootstrap sample has the same number of data points as the original sample. The values of the samples in the bootstrap sample are one possible alternative realization of the original data set. For example, suppose that we have ten measurements of emissions from ten different engines. If we were to randomly sample a different set of ten engines from the same population, we would obtain at least somewhat different values of emissions.

During bootstrap simulation, a large number of bootstrap samples are simulated, typically 500 to 2,000. For each bootstrap sample, one or more statistics of interest may be calculated, such as the mean. Therefore, there will be, typically, 500 to 2,000 estimates of the mean, representing a sampling distribution of mean values. From the sampling distribution, a confidence interval for the mean can be inferred. Similarly, sampling distributions and confidence intervals can be inferred for other statistics, such as the standard deviation, distribution parameters, or percentiles of the cumulative distribution for variability. Results of bootstrap simulation are illustrated later in the paper.

A key advantage of bootstrap simulation for estimation of confidence intervals is that no restrictive assumptions are required regarding normality, as is required to develop confidence intervals using common analytical methods. Thus, bootstrap simulation can be used on a wide variety of problems. The confidence intervals represent lack of knowledge regarding the true values of the statistics being estimated. The confidence intervals have a given confidence level (e.g., 95 percent) of enclosing the true but unknown value of the statistic.

3.0 NATURAL GAS-FUELED INTERNAL COMBUSTION ENGINES

Natural gas-fueled internal combustion engines are commonly used to provide mechanical shaft power to drive compressors, such as those used in natural gas pipelines.[19,20] These engines are classified based upon three major designs: (1) 2-cycle lean burn, also referred to as 2-stroke lean burn (2SLB); (2) 4-stroke lean burn (4SLB); and (3) 4-stroke rich burn (4SRB). Engines in all of these categories are spark-ignited. The capacity of these engines ranges from 50 brake horsepower (bhp) to 11,000 bhp. The air-to-fuel mass ratios of lean burn engines are typically higher than 24:1. Rich burn engines operate near a stoichiometric air-to-fuel mass ratio of 16:1.

Natural gas-fueled engines typically emit nitrogen oxides (NO_x), carbon monoxide (CO), and hydrocarbons (HC). Control technologies for natural gas-fueled engines are primarily aimed at reducing NO_x emissions. Parametric controls involve modifying the spark timing of the engine and/or operating at a leaner air-to-fuel ratio. Combustion modifications are typically aimed at improving the mixing of fuel and air and promoting staged combustion. Examples include clean burn reciprocating head designs and pre-stratified charge combustion. Post-combustion controls include selective catalytic reduction (SCR) for lean burn engines and nonselective catalytic reduction (NSCR) for rich burn engines.[19,20]

Emission factors for natural gas-fueled engines have been published by U.S. EPA in AP-42.[1] Until recently, emission factors for this source category were based upon an October 1996 update to AP-42.[19] However, an update was published in July 2000.[20] The July 2000 version is based upon a different data set than the October 1996 version. The October 1996 data set involves market-share weighted data for at least one of the emission factors. The method for characterizing variability and uncertainty for such data is slightly different than when data are equally weighted. Therefore, to demonstrate a range of methods, both sources of data are included in this study. This study focuses on NO_x and TOC emission factors, because these two pollutants are the most significant precursors to tropospheric ozone formation.

Table 1. Emissions data for Uncontrolled Natural-Gas Fueled 2-Stroke Lean Burn Engines[21]

MAKE	NO_x Emissions ($lb/10^6$ BTU)	TOC Emissions ($lb/10^6$ BTU)	Ratio of total installed capacity (%)
Ajax	1.132	4.318	4
Clark	2.636	1.703	36
CB	3.009	1.164	47
Fairbanks-Morse	0.556	1.220	1
Worthington	2.466	1.618	12
Weighted average	2.710	1.539	

3.1 October 1996 Version of Natural Gas-Fueled Engine AP-42 Emission Factors

In the October 1996 version of AP-42, NO_x and TOC emission factors are provided in four different units: lb/hp-hr; kg/kw-hr; $lb/10^6$ Btu and ng/J. The first two are emissions per unit of engine output, and the last two are emissions per unit of fuel input. The units of $lb/10^6$ Btu are used in this study. The analysis of the October 1996 version is focused upon lean burn engines, because these engines have high emission rates and are present in an airshed (for Charlotte, NC) that is the subject of a case study in related work. The specific emission sources for which uncertainty in average emission factors were quantified include: (1) 2SLB uncontrolled engines; (2) 2-cycle "clean burn" controlled lean burn engines; (3) 2-cycle pre-combustion chamber controlled lean burn engines; and (4) 4SLB uncontrolled engines. For other control options, apparently only one data point was used by EPA to estimate emission factors.[21] Therefore, other control options were not analyzed statistically.

For the 2SLB uncontrolled engines, only average emissions data for each of five manufacturers were available. In addition, the market share for each manufacturer, in terms of the percentage share of installed capacity, was reported. The data set for this type of engine is given in Table 1. As another example of an emission factor data set, the data reported to be used by EPA to calculate the NO_x and TOC emission factors for clean burn 2SLB engines are shown in Table 2. The latter data set is based upon tests done on Copper-Bessemer “Clean Burn” engines.

As a method for verifying whether the data reported in the literature are the complete data set used to develop the AP-42 emission factors, the average value of the data was calculated and compared to the AP-42 value. The weighted average of the uncontolled 2SLB engine emission data was calculated and is provided in Table 1. The weighted average is exactly the same as the AP-42 emission factor in this case. Similarly, the average values of the data in Table 2 are the same as the AP-42 emission factors. Therefore, the data set appears to be exactly the same as that used by EPA in developing the emission factor.

The uncontrolled engine emission factors were assigned a data quality rating of “A” by EPA because they judged that the quantity and quality of the original test data were good and generally well documented, and that the engine types and population profile were known. The Clean Burn and Pre-Combustion Chamber controlled engine emission factors were rated as “C,”

Table 2. Emission data for Clean Burn Natural-Gas Fueled 2-Stroke Lean Burn Engines[21]

Data Point	NO_x Emission Rate ($lb/10^6$ BTU)	TOC Emission Rate ($lb/10^6$ BTU)
1	0.757	0.984
2	0.670	1.019
3	1.534	0.834
4	0.792	0.979
5	0.757	1.005
6	0.675	1.013
7	0.674	1.027
8	0.669	1.029
9	0.873	0.174
10	0.874	0.180
11	0.901	0.190
Average	0.834	0.767

based on a judgment that the test data were of “A” quality, but that the amount of data was limited.[21]

3.2 July 2000 Version of Natural Gas-Fueled Engine AP-42 Emission Factors

After the October 1996 version was published, EPA initiated efforts to gather additional emissions data for combustion sources, including stationary reciprocating internal combustion engines. EPA decided to base the emission factors for natural gas-fueled engines on original emissions source test data.[22] The July 2000 emission factors are only for uncontrolled engines. However, the uncontrolled NO_x emission factors have been refined by estimating emissions separately for two different load ranges. EPA has made publicly available the data used to develop the new emission factors. These data are available in a Microsoft Access database at the EPA TTN web site.[23] A summary of the average emission factor calculated from the data base and of the emission factor reported in AP-42 is given in Table 3.

Two alternative procedures were used to estimate emission factors from the database. In one procedure, referred to in Table 3 as "ungrouped", each data point in the database was given equal weight, even if some of the data represent repeated measurements of the same engine. In the other procedure, referred to as "grouped," all data for a single engine were averaged, and only the average value for each engine was used to calculate an average emission rate. Of the six emission factors shown in Table 3, it appears that for two of them (2SLB NO_x, both load ranges) it is possible to exactly recalculate the AP-42 emission factor from the available data using the "ungrouped" approach. For both of the TOC emission factors it is possible get a very close approximation to the AP-42 value using the ungrouped approach. For the remaining two emission factors (4SLB NO_x, both load ranges), it is not possible to get a reasonable approximation to the AP-42 value using either approach.

Table 3. Comparison Between EPA NO_x Emissions Database and Documentation of AP-42 Emission Factors for Uncontrolled 2SLB and 4SLB Engines Based Upon July 2000 Version of AP-42.[22]

Engine Type	Pollutant	Engine Load	Average Calculated from Database[a] ($lb/10^6$ Btu)	AP-42 Emission Factor ($lb/10^6$ Btu)	Comments on Documentation[b]
2SLB	NO_x	90 to 105%	3.17 (ungrouped), 3.05 (grouped)	3.17	34 test data are used to develop AP-42 emission factor
		< 90%	1.94 (ungrouped), 2.35 (grouped)	1.94	57 test data are used to develop AP-42 emission factor
	TOC[c]	Any load	1.61(ungrouped), 1.49 (grouped)	1.64	24 test data are used to develop AP-42 emission factor
4SLB	NO_x	90 to 105%	2.22 (ungrouped) 3.26 (grouped)	4.08	25 test data are used to develop AP-42 emission factor
		< 90%	0.739 (ungrouped) 1.77 (grouped)	0.847	13 test data are used to develop AP-42 emission factor
	TOC[c]	Any load	1.42(ungrouped), 1.13 (grouped)	1.47	37 test data are used to develop AP-42 emission factor

[a] Two average values were calculated from the available data in the database from the EPA TTN Web Site. The "Ungrouped" averages involve taking the average of all emissions tests for all engines. The "Grouped" averages involve first calculating the average emissions for engines that were tested more than once, and then calculating the average among all engines. For example, if we have 25 test data from 10 engines, the ungrouped average is based upon 25 equally weighted values. In contrast, the grouped average would be based on the 10 average values for each different engine.
[b] The test identification numbers used in the on-line database are documented in Reference 22.
[c] Emission factors are reported on a TOC basis in AP-42. While, they are reported as Total Hydrocarbons (THC) in database.[20,23]

The emission factors of the uncontrolled 2SLB engines are assigned a quality rating “A”, and the emission factors of the uncontrolled 4SLB engines are assigned a quality rating of “B.” However, no explanations regarding the specific basis for these ratings are provided.

Although it was not possible to reproduce the calculation methods for several of the emission factors, the available data are used nonetheless to illustrate the methodology for quantifying uncertainty in emission factors. This case study can be revisited at a later time when documentation of the AP-42 emission factors is more complete.

The July 2000 AP-42 NO_x emission factors differ from the October 1996 AP-42 NO_x emission factors. For example, for uncontrolled 2SLB engines, the October 1996 NO_x emission factor is 2.71 $lb/10^6$ BTU, while the July 2000 emission factor is 3.17 $lb/10^6$ BTU for the 90 percent to 105 percent load range. For the less than 90 percent load range, the July 2000 emission factor is 1.94 $lb/10^6$ BTU. It is not known for what load range the October 1996 data were obtained. However, it appears that the October 1996 average emission factor is enclosed by the range of emission factors in the July 2000 version. The comparison of 4-cycle uncontrolled lean burn engine emission factors is similar. The October 1996 NO_x emission factor of 3.2 lb/10^6 BTU is enclosed by the July 2000 values of 4.1 lb/10^6 BTU for the high load range and 0.85 lb/10^6 BTU for the low load range. The October 1996 TOC emission factors were 1.539 lb/10^6 BTU for 2SLB engines and 1.261 lb/10^6 BTU for 4SLB engines. In July 2000 version AP-42, these emission factors are approximately comparable with values of 1.64 lb/10^6 BTU for 2SLB engines and 1.47 lb/10^6 BTU for 4SLB engines.

4.0 QUANTIFICATION OF VARIABILITY AND UNCERTAINTY IN EMISSION FACTORS

In this section, variability in the emission factor data sets is represented with parametric probability distributions. Uncertainty in the average emission factors is estimated using bootstrap simulation. Two sets of case studies are presented. In the first case study, each data point is assumed to be an equally likely random sample from the total population of emission sources. This type of case study applies to all of the emission factor data except for the October 1996 version uncontrolled 2SLB engine data. In the latter case, each data point does not have equal weight. Therefore, the uncertainty estimation method is modified to attempt to account for the unequal weights of each data point.

4.1 Equally-Weighted Randomly Sampled Data

In many cases, emission factor data are available for a sample of engines, representing different manufacturers, engine models, engine ages, applications, etc. In developing an emission factor, a judgment is made to group data from various specific engine measurements together because of similarities in engine design and operation. For example, expert judgment could be used as a basis for estimating the market share of each particular make and model of engine. In the absence of information, a common default assumption is to assume equal weight among the available data. Of course, this assumption could, and is likely to, be wrong. At the same time, there may not be an empirical basis to justify other assumptions. Key assumptions in an analysis should be evaluated when interpreting the results of the analysis. Therefore, although equal weight for each data point is assumed, later this assumption will be critiqued.

Another factor that must be considered is how to handle replicate data. The available data sets include, in some cases, repeated measurements on the same engine. For example, in the case of the July 2000 data set for uncontrolled NO_x emissions from 4SLB engines operated at 90 percent to 105 percent load, there are 25 data points available from measurements on only 5 engine models. Repeated measurements on the same engine provide an indication of intra-engine variability in emissions. However, in calculating an emission factor, the objective is to quantify inter-engine variability in emissions for purposes of estimating the population distribution for variability within the source category. Therefore, it is necessary to prepare a data set representative of inter-engine variability. The approach taken here is to use an average value for repeated measurements of an individual engine as the representative emission rate for that engine, and to analyze the inter-engine variability in which each engine is represented by either one data point, if only one measurement is available, or the average of the available data, if repeated measurements are available.

Table 4. Summary of Emission Test Data Using in July 2000 Version of AP-42 for Uncontrolled 4SLB Engines Operated at 90 to 105 Percent of Load.

Engine Make and Model	Engine Size (hp)	Engine Load Range (%)	Number of Tests	Range of Test Results ($lb/10^6$ BTU)	Average Emissions ($lb/10^6$ BTU)
Caterpillar G339T	850	100	1	2.11	2.11
Cooper-Bessemer LSV-16	4,200	98-99	4	2.41 to 3.28	2.90
Ingersoll Rand KVS-412	2,000	91	2	5.24 to 5.63	5.44
Ingersoll Rand KVS-12	2,000	100	5	4.98 to 6.01	5.65
Waukesha 3521 GL	736	100	13	0.11 to 0.38	0.21

As an example to illustrate the development of an emission factor database, Table 4 summarizes the NO_x emission data for five uncontrolled 4SLB engines operated at 90 to 105 percent load. However, it appears that the Ingersoll Rand KVS-412 and KVS-12 engines might be the same engine; they have the same rated capacity and very similar emission factors. Nonetheless, for the time being, these are treated separately because they are reported separately in the data base and there is no evidence in the AP-42 supporting documentation that EPA treated them as the same engine in developing the AP-42 emission factors.[22] In the future, this data set should be revisited or more thoroughly documented to clarify this point. Although there are a total of 25 measurements in the database, because the measurements are for only five engines, the effective sample size is only five. The variability in emissions for a single engine is less than the variability in emissions between engines. For example, the range of variation in emissions for the Cooper Bessemer LSV-16 engine over four measurements is approximately plus 0.4 $lb/10^6$ BTU or minus 0.5 $lb/10^6$ BTU from an average of 2.90 $lb/10^6$ BTU. However, the range of variation when comparing engines is from 0.2 $lb/10^6$ BTU to 5.7 $lb/10^6$ BTU, or a factor of nearly 30. Thus, although there is variability in emissions for an individual engine, the inter-engine variability is substantially larger.

The inter-engine variability in emissions for the uncontrolled 4SLB engines is shown graphically in Figure 1. Of the several types of parametric distributions evaluated, the Weibull distribution offered the best fit to the five data points. With only five data points, there are not sufficient data to perform statistical goodness-of-fit tests. Bootstrap simulation was used to estimate confidence intervals for the CDF of the fitted parametric distributions. With only five data points, the confidence intervals are relatively wide. For example, the 95 percent confidence interval for the median, or 50th percentile of the distribution, is from 1.07 $lb/10^6$ BTU to 5.41 $lb/10^6$ BTU, which is nearly as wide as the range of the data.

The mean emission rate calculated from the original data set using groupings by engine is 3.26 $lb/10^6$ BTU. The mean emission estimate obtained from the fitted distribution is 3.17 $lb/10^6$ BTU. The difference is because the fitted distribution places less emphasis on larger values of emissions than the data set, which has two values of relatively high emissions. The 95 percent confidence interval for the mean is from 1.36 $lb/10^6$ BTU to 5.73 $lb/10^6$ BTU, corresponding to a range of minus 57 percent to plus 81 percent. The AP-42 emission factor is 4.08 $lb/10^6$ BTU. The mean emission estimate from bootstrap simulation is 22 percent smaller than than the AP-42 value, although the confidence interval encloses the AP-42 value. However, insufficient documentation of the AP-42 value is provided to enable more detailed comparisons.

Figure 1. Comparison of Empirical Cumulative Distribution of Average Uncontrolled 4-SLB Engine, 90-105% load, NO_x Emissions, fitted Weibull distribution, and Bootstrap Simulation Confidence Intervals, Based Upon July 2000 AP-42 Data.

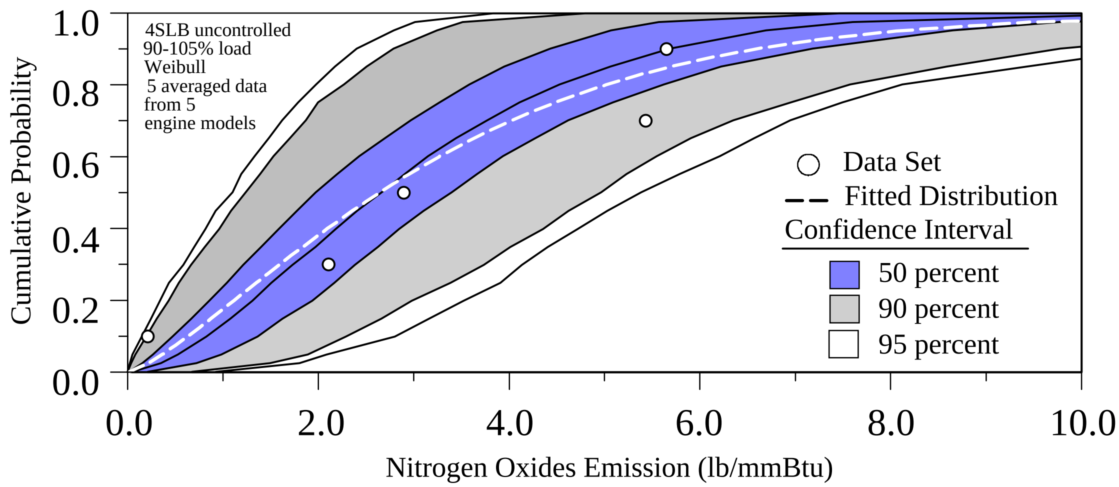
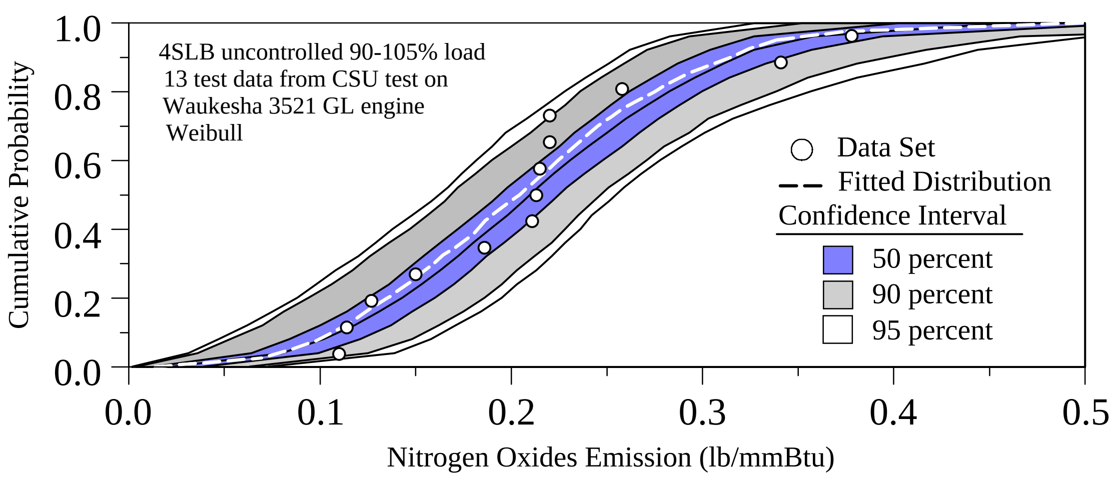


Figure 2. Comparison of Empirical Cumulative Distribution of Uncontrolled Waukesha 3521 GL 4SLB Engine, 90-105% load, NO_x Emissions, a fitted Weibull distribution for Intra-Engine Variability and Bootstrap Simulation Confidence Intervals, Based Upon July 2000 AP-42 Data.



An important characteristic of the confidence intervals of the mean, or of any other statistic, estimated based upon bootstrap simulation is that they need not be symmetric. With a very small data set of only five data points, and with a positive skewness in the data set, the confidence interval on the mean is expected to be positively skewed. Therefore, the asymmetry of the confidence interval for the mean NO_x emission factor from 4SLB engines is expected. Because of the small number of data points and the wide range of variability of the data, the confidence interval is expected to be relatively wide, as it is in this case.

The adequacy of the fitted distribution can be evaluated, at least in part, by identifying what proportion of the data are contained with the confidence intervals of the CDF. On average, if the fit is a good one, half of the data should be enclosed within the 50 percent confidence interval, 90 percent of the data should be enclosed within the 90 percent confidence interval, and 95 percent of the data should be enclosed within the 95 percent confidence interval. In Figure 1, three of the five data points are contained within the 50 percent confidence interval, and all of the data are enclosed by the 90 percent confidence interval. This suggests, though cannot prove, that the Weibull distribution is an acceptable fit to the data.

An example of intra-engine variability in emissions is shown in Figure 2, based upon 13 measurements on a Waukesha 3521 GL engine at 100 percent load. A Weibull distribution was chosen as the best fit to the data. The mean estimate obtained from the fitted distribution is 0.21 lb/10^6 BTU, with a 95 percent confidence interval from 0.17 lb/10^6 BTU to 0.25 lb/10^6 BTU, corresponding to a range of minus 21 percent to plus 19 percent. In this case, the intra-engine variation in emissions is much smaller than the inter-engine variability in emissions.

Probabilistic analysis results for the case of uncontrolled 2-SLB engine NO_x data, based upon the July 2000 AP-42 data, are given in Figure 3 and Figure 4 for the high load (90 to 105 percent) and low (<90 percent) load ranges, respectively. Figure 3 illustrates that the fitted Weibull distribution agrees very well with the eleven data points; ten of eleven values are enclosed by the 50 percent confidence interval. The data shown in Figure 4 appear to be in two groups: one group of data are less than 1.5 lb/10^6 BTU, and another group is greater than 3.5 lb/10^6 BTU. Half of the data points are enclosed by the 50 percent confidence interval, and all of the ten data points appear to be enclosed by the 90 percent confidence interval. However, it is clear that the fit is influenced by the grouping of the data. While it may be the case that a mixture distribution would be a better fit, it is difficult to fit mixture distributions to such a small data set.

Figure 3. Comparison of Empirical Cumulative Distribution of Average Uncontrolled 2-SLB Engine 90-105% load, NO_x Emissions, fitted Weibull distribution, and Bootstrap Simulation Confidence Intervals, Based Upon July 2000 AP-42 Data.

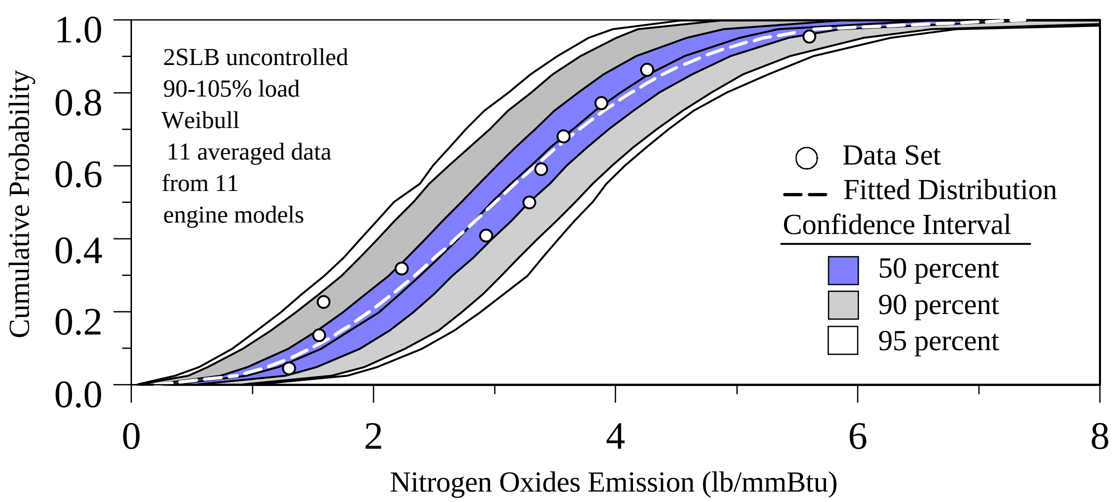
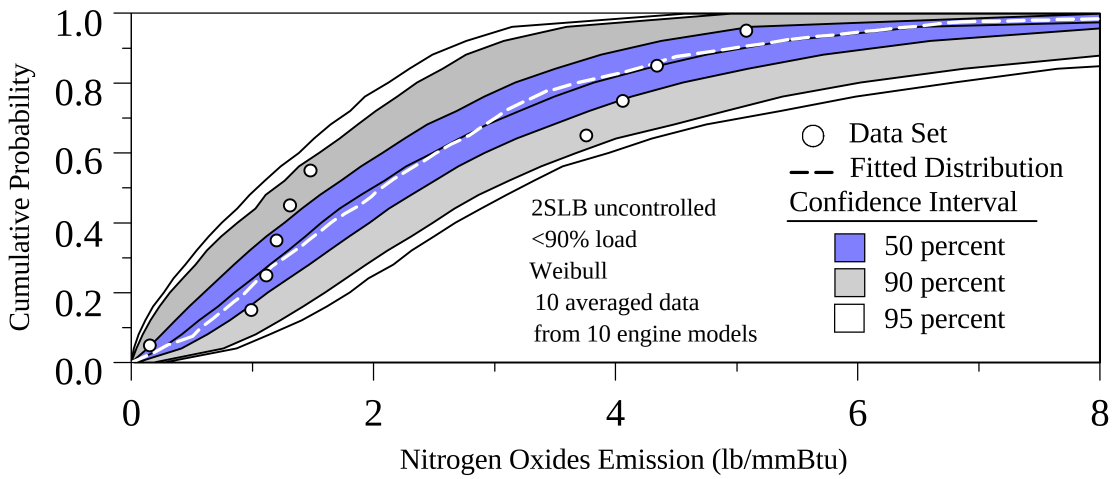


Figure 4. Comparison of Empirical Cumulative Distribution of Average Uncontrolled 2-SLB Engine <90% load, NO_x Emissions, fitted Weibull distribution, and Bootstrap Simulation Confidence Intervals, Based Upon July 2000 AP-42 Data.



4.2 Unequally-Weighted Data

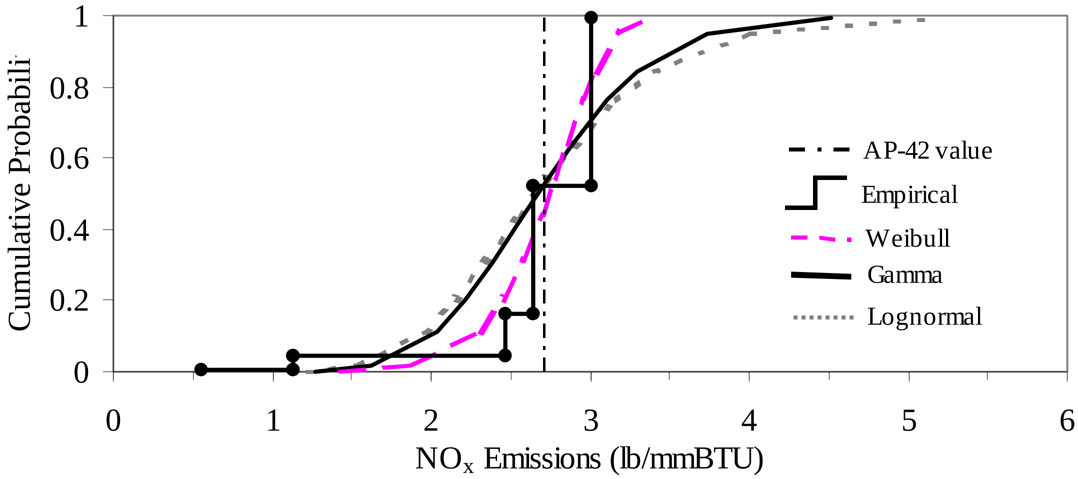
In this section, an example case study is presented based upon emissions data that are not equally weighted. These data are from Table 1 for uncontrolled 2SLB engines, based upon the October 1996 version of AP-42. The five emissions values are shown in Figure 5 as an empirical CDF, along with three parametric distributions that have been fit to the data.

Because each of the five emissions values has a different market share-based weight, the method for fitting distributions to the data had to be modified compared to when data have equal weight. The approach taken here was to use 100 synthetic data points as a basis. The use of 100 basis data points allows for emission values to occur repeatedly in proportion to their market share. A portion of these 100 data points were assigned the emission factor associated with an engine, in proportion to the market share of that engine. For example, the Clark engines have 36 percent of the market share; therefore, 36 of the 100 basis data points were assigned the Clark engine emission value of 2.64 lb/10^6 BTU. Parametric distributions were fit to the 100 basis data points.

The comparison of the fitted distributions in Figure 6 suggests that the Weibull distribution may provide the best fit to the data. The Weibull distribution provides the best fit in the central portion of the distribution, and appears not to have as "heavy" of a tail at the upper end of the distribution. For comparison purposes, both the Weibull and Lognormal distributions are included in the bootstrap simulation analyses, the results of which are given in Figures 6 and 7.

In the bootstrap simulation, the number of bootstrap samples was 500, and the number of data points per bootstrap sample was five. During bootstrap simulation, each simulated data point has equal weight. However, because the parametric distributions were fit to market share-weighted data, the shape of the parametric distributions reflects the frequency with which data should be sampled in different emission ranges. For example, the steepness of the fitted CDF in the range

Figure 5: Empirical Distribution and Fitted Parametric Distributions for Market-Share Weighted NO_x Emissions Rates for Uncontrolled 2-Cycle Lean Burn Engines Based Upon October 1996 AP-42 Data



from approximately 2 lb/10^6 BTU to 3 lb/10^6 BTU means that there is a high probability that random samples of emissions will occur in this range, corresponding to the three engines that have the largest combined market share. In contrast, there is comparatively little probability that emissions values will be sampled for the two engines that, together, comprise only five percent of the total market share.

The results of the bootstrap simulation with the Lognormal distribution are given in Figure 6. It appears that the 95 percent confidence interval encloses the empirical distribution of the data. However, the confidence intervals are very wide, and there appear to be biases in the fit. For example, the central range of the empirical distribution coincides with the high side of the confidence intervals, while the lower and upper tails of the empirical distribution coincide with the low side of the confidence interval. The apparent biases in the fit, and the wideness of the

Figure 6. Comparison of the Empirical Distribution Bootstrap Simulation Results Based Upon a Lognormal Distribution for Market-Share Weighted NO_x Emissions Rates for Uncontrolled 2-Cycle Lean Burn Engines Based Upon October 1996 AP-42 Data

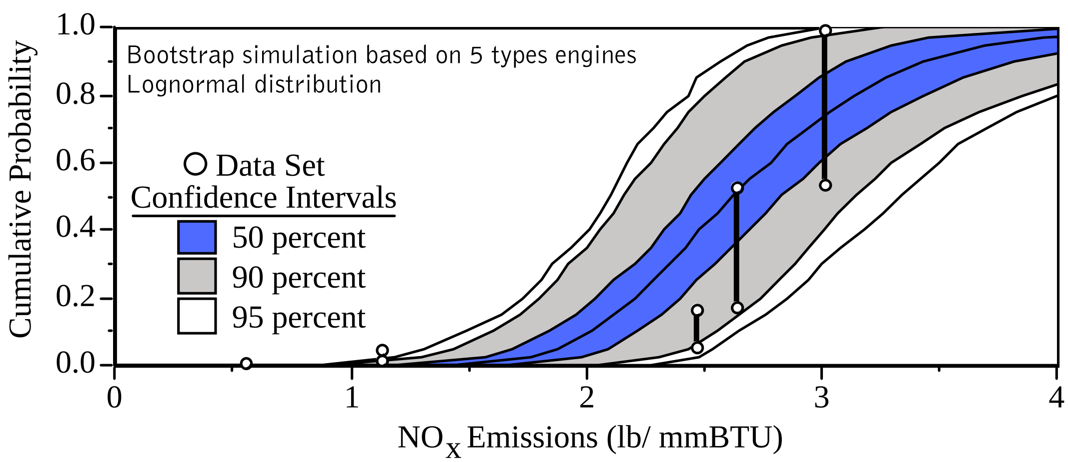
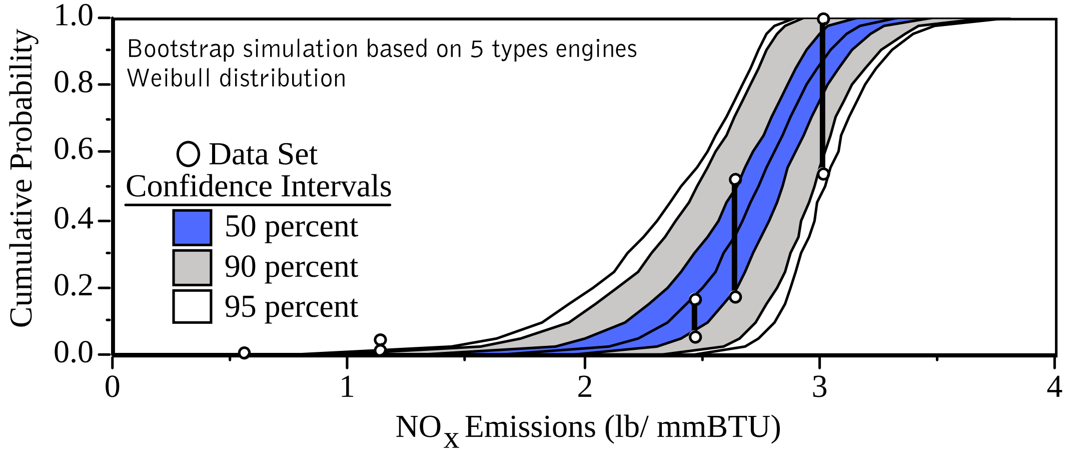


Figure 7. Comparison of the Empirical Distribution Bootstrap Simulation Results Based Upon a Weibull Distribution for Market-Share Weighted NO_x Emissions Rates for Uncontrolled 2-Cycle Lean Burn Engines Based Upon October 1996 AP-42 Data



intervals, suggest that the Lognormal is not a particularly good distribution to use in this case.

The results of the bootstrap simulation with the Weibull distribution are given in Figure 7. These results imply more consistency between the assumed parametric distribution and the empirical distribution of the original data. In particular, the empirical distribution appears to be reasonably well enclosed by the 90 percent confidence interval, and the width of the confidence interval is much narrower compared to the Lognormal case, without compromising the apparent goodness-of-fit. Therefore, the Weibull distribution is selected over the Lognormal distribution as a more appropriate basis for estimating uncertainty in the mean. The choice of parametric distribution influences the estimated confidence interval for the mean. The 95 percent confidence interval for the mean is 2.14 to 3.38 lb/10^6 BTU based upon the Lognormal distribution, 2.25 to 3.26 lb/10^6 BTU based upon the Gamma distribution, and 2.39 to 2.99 lb/10^6 BTU based upon the Weibull distribution. Of these three, the Weibull distribution leads to the narrowest estimate of the confidence interval.

5.0 Summary of Probabilistic Estimation Results for AP-42 October 1996 Version and July 2000 Version Emission Factors

A summary of probabilistic estimations of uncertainties in emission factors for uncontrolled natural gas pipeline compressor engines are presented in Table 5, 6, 7 and 8. For the October 1996 version, the analysis is based upon the complete dataset used by EPA to develop the AP-42 emission factors. For the July 2000 version, the methods used by EPA were not fully documented. However, the relative range of uncertainty estimated for these emission factors may still be useful in characterizing uncertainty.

Table 5. 95 Percent Confidence Interval for Mean NO_x Emissions for Natural Gas-Fueled Internal Combustion Lean Burn Engines, Based on October 1996 AP-42 Data

Engine and Emissions Control Technology	No. of Data	Mean of Data[a]	AP-42 Emission Factor[a]	Fitted Distrib.	Mean of Bootstrap Sample Means[a]	Relative 95% CI on Mean[b]
2SLB, Uncontrolled	5	2.710	2.710	Weibull	2.714	-11.8% to +9.36%
2SLB, Clean Burn	11	0.834	0.834	Lognormal	0.835	-14.1% to +15.4%
2SLB, PCC[c]	20	0.850	0.850	Lognormal	0.840	-23.7% to +28.5%
4SLB, Uncontrolled	4	3.225	3.225	Weibull	3.170	-27.2% to +30.8%

[a]Units are lb/10^6 BTU. [b]Calculated based upon bootstrap simulation results. [c]PCC=Pre-Combustion Chamber

Table 6. 95 Percent Confidence Intervals for Mean TOC Emissions for Natural Gas-Fueled Internal Combustion Lean Burn Engines, Based on October 1996 AP-42 Data

Engine and Emissions Control Technology	No. of Data	Mean of Data[a]	AP-42 Emission Factor[a]	Fitted Distrib.	Mean of Bootstrap Sample Means[a]	Relative 95% CI on Mean[b]
2SLB, Uncontrolled	5	1.539	1.539	Weibull	1.549	-36.0% to +42.7%
2SLB, Clean Burn	11	0.767	0.767	Weibull	0.770	-56.1% to +67.5%
2SLB, PCC[c]	20	1.756	1.756	Weibull	1.750	-17.1% to +18.3%
4SLB, Uncontrolled	4	1.261	1.261	Weibull	1.278	-47.6% to 55.7%

[a]Units are lb/10^6 BTU. [b]Calculated based upon bootstrap simulation results. [c]PCC=Pre-Combustion Chamber

Table 7. 95 Percent Confidence Intervals for Mean Uncontrolled NO_x Emissions for Natural Gas-Fueled Internal Combustion Lean Burn Engines, Based on July 2000 AP-42 Data

Engine and Load Range	AP-42 Emission Factor[a]	No. of Data	No. of Engines	Fitted Distrib.	Mean of Bootstrap Sample Means[a]	Relative 95% CI on Mean[b]
2SLB, 90% to 105%	3.17	34	11	Weibull	3.05	-24% to +24%
2SLB, < 90%	1.94	24	10	Weibull	2.41	-44% to +53%
4SLB, 90% to 105%	4.08	25	5	Weibull	3.17	-57% to +81%
4SLB, < 90%	0.847	13	4	Weibull	1.65	-84% to +165%

[a]Units are lb/10^6 BTU. [b]Calculated based upon bootstrap simulation results.

Table 8. 95 Percent Confidence Intervals for Mean TOC Emissions for Natural Gas-Fueled Internal Combustion Lean Burn Engines, Based on July 2000 AP-42 Data

Engine and Load Range	AP-42 Emission Factor[a]	No. of Data	No. of Engines	Fitted Distrib.	Mean of Bootstrap Sample Means[a]	Relative 95% CI on Mean[b]
2SLB, Uncontrolled	1.64	57	14	Weibull	1.45	-16% to +18%
4SLB, Uncontrolled	1.47	37	4	Weibull	1.10	-51% to +50%

[a]Units are lb/10^6 BTU. [b]Calculated based upon bootstrap simulation results.

The summary tables indicate that the 95 percent range of uncertainty in the mean emission factor ranges from as low as approximately plus or minus 10 percent to as high as minus 84 to plus 165 percent. The range of uncertainty is influenced by a combination of the sample size and the range of variability in the data. Smaller sample sizes and/or larger inter-engine variability in the data will tend to contribute to wider ranges of uncertainty in the estimated mean emission factor.

6.0 DISCUSSIONS AND CONCLUSIONS

This paper demonstrates the successful application of quantitative probabilistic analysis to emission factor case studies, based upon the example of stationary natural gas-fueled internal combustion engines. The method employed is based upon characterization of uncertainty based upon random sampling error. The method includes: (1) development of a database; (2) visualization of the data using empirical CDFs; (3) evaluation of alternative parametric probability distributions fitted to the data; (4) bootstrap simulation to characterize confidence intervals in the fitted CDF; (5) selection of a judged best fit distribution based upon bootstrap simulation results; and (6) quantification of uncertainty in the mean based upon the bootstrap sampling distribution for the mean.

The probabilistic method was applied to several different types of analyses, including: (1) quantification of inter-engine variability in emissions and uncertainty in the mean for unequally weighted data points; (2) quantification of inter-engine variability in emissions and uncertainty in the mean for equally weighted data points; and (3) quantification of intra-engine variability in emissions and uncertainty in individual engine emissions, based upon repeated measurements of a single engine. The range of inter-engine variability in emissions was typically as low as a factor of five or as large as a factor of almost 30. The range of intra-engine variability in emissions was typically much smaller on an absolute basis than the range of inter-engine variability. The range of inter-engine variability in emissions suggests that the weights assigned to each engine emission estimate can significantly affect the estimate of the mean emission rate. Thus, the assumption of equal weighting of emissions data, as is often made, is likely to be a strong assumption in many cases and, therefore, can be a significant factor biasing emission factor estimates.

The estimates of uncertainty in the mean are often asymmetric, indicating that skewness regarding observed variability in inter-engine emissions can lead to skewness in the estimate of uncertainty in the mean. Conventional analytical methods based upon normality assumptions can lead to errors in the uncertainty estimate. The mean values estimated from the probabilistic analysis differ in some cases from the mean values estimated directly from the data because parametric probability distributions allow for interpolation within the range of observed data and for extrapolations beyond the range of observed data. For small data sets, it is unlikely that the observed sample of data truly includes the minimum and maximum possible values. On this basis, extrapolation is warranted.

Although three parametric distributions were typically evaluated, most often the Weibull distribution was found to provide a good fit to the data. The Weibull may take on many shapes, including negatively skewed, symmetric, or positively skewed. Furthermore, the Weibull distribution also tends to be less "tail-heavy" than the other two, and often provides a better empirical fit to the data for these reasons.

The quantitative analysis demonstrated here focuses on one important source of uncertainty. The range of uncertainty associated with random sampling error was found to be as large as minus 84 percent to plus 165 percent, and in most examples was greater than plus or minus 20 percent. Some other sources of uncertainty, such as potential lack of representativeness of the test cycles used in the measurements, or potential lack of representativeness of the sample of engines, are difficult to evaluate quantitatively. Therefore, it is recommended that qualitative methods for identifying sources of uncertainty *also* be used. However, there is not a direct relationship between the qualitative data rating and the range of uncertainty in the emission factor. Therefore, we do not recommend that data quality ratings be used to make inferences regarding quantitative ranges of uncertainty.

A significant difficulty encountered in this study was the lack of documentation of the calculation methods for the July 2000 AP-42 emission factors. Complete documentation should include enough information so that others can reproduce the calculations and results. Therefore, we recommend that EPA report the complete calculation method used for each emission factor. With the growing recognition of the importance of quantitative uncertainty analysis, it will be important for EPA and others to routinely report data regarding variability and uncertainty in emission factors.

7.0 ACKNOWLEDGEMENTS

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KEY WORDS
Emission factors, NO_x, TOC, Uncertainty, Variability, Bootstrap simulation, Emissions, Inventories, Engines, Probabilistic Analysis, Monte Carlo simulation.