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MODELING AIR TOXICS EMISSIONS FROM ELECTRIC POWER PLANTS

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ABSTRACT

This paper describes a power plant chemical assessment model being developed for the Electric Power Research Institute (EPRI) as part of its air toxics program. The model provides probabilistic estimates of trace species emissions based on user-specified plant and fuel characteristics, drawing on a database of published information on trace species partitioning characteristics. The results of two case studies are presented in which emission estimates from the probabilistic model are compared to experimental values for two coal-fired power plants. The case studies illustrate a high degree of uncertainty in trace species emission estimates, and underscore the need for additional data acquisition, combined with a probabilistic representation of results.

INTRODUCTION

The U.S. Environmental Protection Agency is considering the possibility of regulations regarding potentially toxic air emissions from electric utility power plants. This has motivated research aimed at understanding and characterizing trace species emissions from a variety of power plant systems. This paper focuses on the development and application of a power plant chemical assessment model. This model allows electric utilities to evaluate the performance of a given power plant configuration with respect to multi–media emissions of chemical substances. The model provides estimates of the mass flow rates of all solid, liquid and gaseous streams emanating from the plant, including quantitative estimates of all trace species emissions.

A unique feature of the model is its ability to characterize uncertainties probabilistically. Any or all model input parameters can be assigned a probability distribution rather than a single value. The combined effect of all input uncertainties (obtained using Monte Carlo methods) then is reflected in an uncertainty distribution for output parameters of interest. Such distributions indicated both the range and likelihood of possible values, in contrast to conventional single–valued estimates. The model can be run using either deterministic values or uncertainty distributions yielding probabilistic results.

Descriptions of the initial model development and applications have been reported previously[1, 2]. Here, we briefly summarize the model structure and design, then elaborate on recent case studies that illustrate applications of the model to potential air toxics and related assessments.

THE REGULATORY IMPERATIVE

The Clean Air Act Amendments (CAAA) of 1990 gave new importance to the control of hazardous air pollutants. Under previous Clean Air Act provisions (Section 112) hazardous pollutants were identified and regulated based on a determination of harm by the U.S. Environmental Protection Agency (EPA). To date, fewer than ten species have been regulated in this manner. Now, 189 chemical species have been named in the new CAAA provisions for air toxics (Title III). Control is required across a broad spectrum of industrial and other sources emitting 10 tons per year (tpy) or more of any one of the listed substances, or 25 tpy or more of any combination of these substances. The basis for regulation is the use of "maximum available control technology" (MACT). Additional controls could be required if EPA finds an unacceptable level of remaining risk to public health after MACT is applied.

Electric utilities are not initially subject to these new air toxics requirements. Still, the CAAA requires EPA to perform several studies of the risks that may occur from emissions of hazardous air pollutants from electric steam generating units, and to regulate electric utilities under Title III if "appropriate and necessary" after considering the results of these studies. Implications of the CAAA on the electric utility industry are summarized elsewhere [3].

In light of possible regulatory developments, the Electric Power Research Institute (EPRI) has undertaken a program to study trace species emissions of utilities and their control. The EPRI program — known as PISCES (Power Plant Integrated Systems: Chemical Emissions Study) — has several major products and activities, including a database of published information on trace species for conventional fossil fuel power plants, a field monitoring program to collect new data, and the probabilistic computer model described in this paper.

MODEL OVERVIEW

The power plant simulation model allows any conventional fossil–fueled power plant to be configured for analysis. Version 1 is limited to conventional coal, oil and gas–fired plants. The model employs fundamental mass and energy balances to compute all system flow rates. Empirical data are employed where necessary to calculate system emissions.

The model requires two types of data. The first involves parameters specifying the power plant configuration and performance. The second involves trace chemical substance data for evaluating trace emissions. The latter includes information on the concentration of trace species in all plant input streams (including fuel, reagents, water, and air), plus performance data characterizing how each chemical constituent in a given stream is "partitioned" or removed in various plant components or environmental control systems.

If a probabilistic analysis is to be performed, plant characteristics, chemical species input quantities, and environmental control system performance characteristics must be specified probabilistically. The PISCES database provides most of the information needed for trace species analysis. To simplify the use of the model, including interaction with the database, a graphical interface has been developed. A detailed description of the model appears elsewhere [4].

MODEL APPLICATIONS

Effective use of the model for trace species evaluation and control strategy depends strongly on the availability of auxiliary data to quantify the various partition factors needed to track chemical species. These partition factors are used to predict the trace species emissions resulting from the particular case study input stream concentrations. In this paper, we illustrate how partition factors from the PISCES database were used with the model for two case studies. These case studies quantify the measured emissions of trace species from two coal-fired power plants.

The case studies were performed using the model, PISCES database, and specific plant data to analyze two power plants located in the eastern United States. These plants are among several sites at which EPRI is acquiring additional field test data on trace species emissions as part of the PISCES program. The model input parameters provided by the utility and field test data are summarized in Table 1. All other model performance parameters utilized model defaults. Of particular interest in the case studies are comparisons between the new test data and estimates based on the previously published studies compiled in the PISCES database.

Case I: A Coal-fired Power Plant with no FGD

The plant configuration of the first plant study consisted of a tangential fired boiler and a cold-side electrostatic precipitator (ESP). The plant burns a low sulfur bituminous coal. Three measured coal samples provided the data used for this analysis. Coal concentration data for some species were reported as less than a specified detection limit, which indicates that the concentration falls between zero and the reported limit. For analysis purposes, data

Table 1. Plant and fuel input parameters for the case studies.

Plant Characteristics	Coal Characteristics (as fired)	Reagent Characteristics
Plant Capacity, MW	HHV, Btu/lb	Trace Species (ppmw)
Steam Cycle Heat Rate, Btu/kWh	Carbon, wt %	
Boiler Efficiency, %	Hydrogen, wt %	
Capacity Factor, %	Oxygen, wt %	
Boiler Excess Air, %	Sulfur, wt %	
Air Preheater Leakage, %	Nitrogen, wt	
Furnace Type	Moisture, wt %	
Ash to Flue Gas, wt %	Ash, wt %	
ESP Ash Removal Efficiency, %	Trace Species (ppmw)	

for these species was omitted from the case study. All power plant performance parameters were treated deterministically using data provided by the host utility.

<u>Plant Performance.</u> Flow rates of the major streams in a power plant determine the magnitude of trace species emissions. Therefore, the plant performance parameters specified in the first column of Table 1 were used to model key plant flow rates.

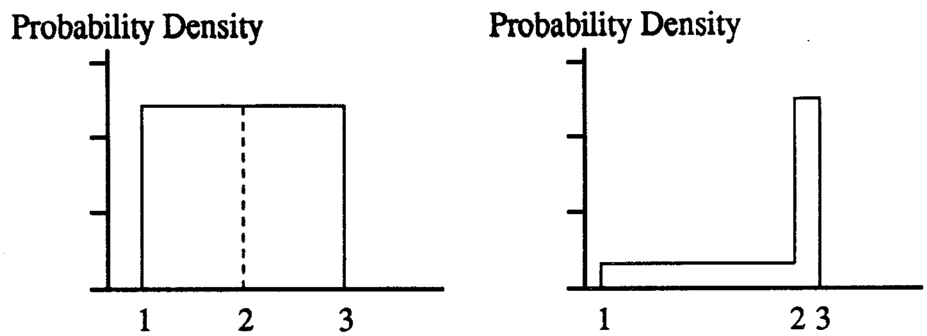
The coal flow rate is determined by the plant capacity, steam cycle heat rate, boiler efficiency, and coal higher heating value (HHV). The coal flow rate calculated by the model using plant parameters supplied by the utility agreed well (within 0.7%) with the flow rate measured during the PISCES field test. The ash flow rate calculation is much simpler, based solely on the coal flow rate, ash content of the coal, and the percentage of ash reporting to the flue gas. The ash flow rates calculated by the model also matched well those measured for the bottom ash, collected fly ash, and emitted ash.

The flue gas flow rate is calculated by the model from the coal combustion products, temperature, excess air to the furnace, air preheater leakage, and downstream leakage. As a secondary check, the oxygen content of the emitted flue gas can be compared. The flow rate and oxygen content initially calculated by the model were consistently lower than the measured values. The apparent discrepancy was reconciled when excess oxygen data revealed a 20% air leakage downstream of the air preheater, of which the utility was not aware. This leakage was later confirmed by the measuring team.

In brief, the major stream flow rates measured during the PISCES field test were consistent with the rates predicted by the model. The only addition to the data supplied by the utility was an additional air leakage term revealed by the measured oxygen content and flow rate of the flue gas.

<u>Trace Performance.</u> The data for trace species concentration in coal were represented by probability distributions. There were a maximum of three measured data points for each trace species in the coal. As an approximation, the range of possible values for trace species concentration was assumed to bounded by the upper and lower measured values. Thus, when only two data points were available, a uniform distribution was employed to represent uncertainty. When three data points were available, a fractile distribution was employed. In estimating the parameters of the fractile distribution, it was assumed that there was an equal probability that the trace species concentration could be above or below the central measured value, bounded by the upper and lower measured values. Figure 1 illustrates fractile probability distributions using three data points that are equally and unequally

Figure 1. Examples of probability density for three data points using a fractile distribution: (a) equally spaced points 1,2 and 3; and (b) unequally spaced points, with 2 and 3 very similar.



spaced.

Additional information was needed to estimate the partitioning of trace species in the furnace and ESP. This information was obtained from the PISCES database. The species partition factors for the furnace were based on roughly a dozen data points from plants burning bituminous coal. Data was used only from plants reporting values for the total ash content of coal, as well as values for the concentration of the trace species in both the coal and bottom ash streams. The ESP partition factor (removal efficiency) was based on roughly a dozen data points from bituminous coal-fired power plants. Both sets of partition factors were represented by fractile distributions.

Given the data and assumptions outlined above, the computer model was used to predict the probabilistic mass flow rates and concentrations of trace species in the coal, bottom ash, collected flyash, and stack gas. All probabilistic results were generated using median Latin Hypercube sampling, which is a more efficient sampling technique than traditional random Monte Carlo simulation [5]. A sample size of 200 was used for the stochastic simulation.

Several trace species not detected in the coal (cadmium, copper and molybdenum) were not modeled. For arsenic, mercury and selenium, the PISCES database did not have sufficient information to calculate furnace partition factors for tangential fired boilers burning bituminous coal. These three volatile trace species were given a furnace partition of unity, resulting in 100% partitioning to the flue gas. This is a conservative assumption with respect to flue gas emissions of these species.

Analysis. Figure 2 shows the probabilistic flow rates of trace species in the emitted flue gas. The solid curves in Figure 2 is the cumulative distribution function (cdf) for the calculated emissions of each species. The cdf represents the likelihood of finding a value at or below a specific reference number. For example, the cobalt emission graph shows a 75% probability of being less than 0.15 pounds per hour or, conversely, a 25% probability of being greater than 0.15 pounds per hour (up to a maximum of approximately 0.6 pounds per hour). The cdf can also be used to identify the probability of measurements falling within a range of values. A black square indicates the mean of the measured values obtained from field studies. The brackets (error bars) around the black squares indicate the 95% confidence interval reported for the data, assuming a normal distribution for the measurements. The region of overlap between measured and calculated values is shown by the area shaded in gray. On the horizontal axis, the range of values represents the 95 percent confidence interval for the measurements. On the vertical axis, the height of the gray region corresponds to the probability that values from the database are less than or equal to the upper confidence limit of the measured value. Figure 2 shows the six

Table 2. Mass balance closure for case study measurements. Cadmium, copper and molybdenum were not calculated because measured coal concentrations were below detection limits.

Species		As	Ba	Be	Cl	Cr	Co	Fl	Pb	Mn	Hg	Ni	P	Se	V
Closure (%)	Case I	65	74	98	70	77	106	65	280	109	26	NC	101	78	97
	Case II	73	79	110	48	74	119	985	143	104	46	49	NC	86	98

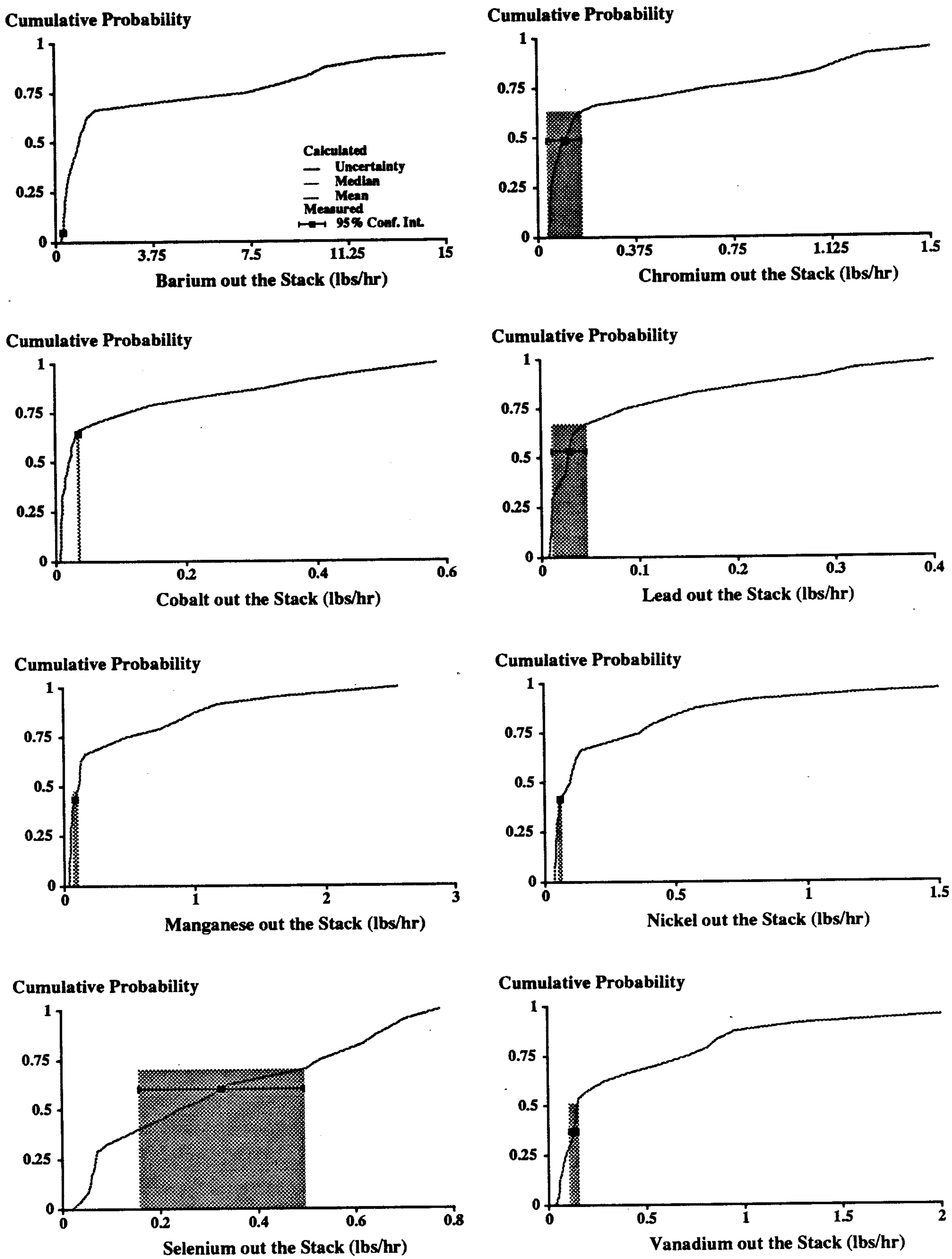


Figure 2. Stack emissions for Case I showing reasonable to good agreement. Measured ranges are based on a normal distribution. Calculated curves are based on fractile distributions of coal measurements and PISCES database partition factors. Regions of overlap are shown in gray.

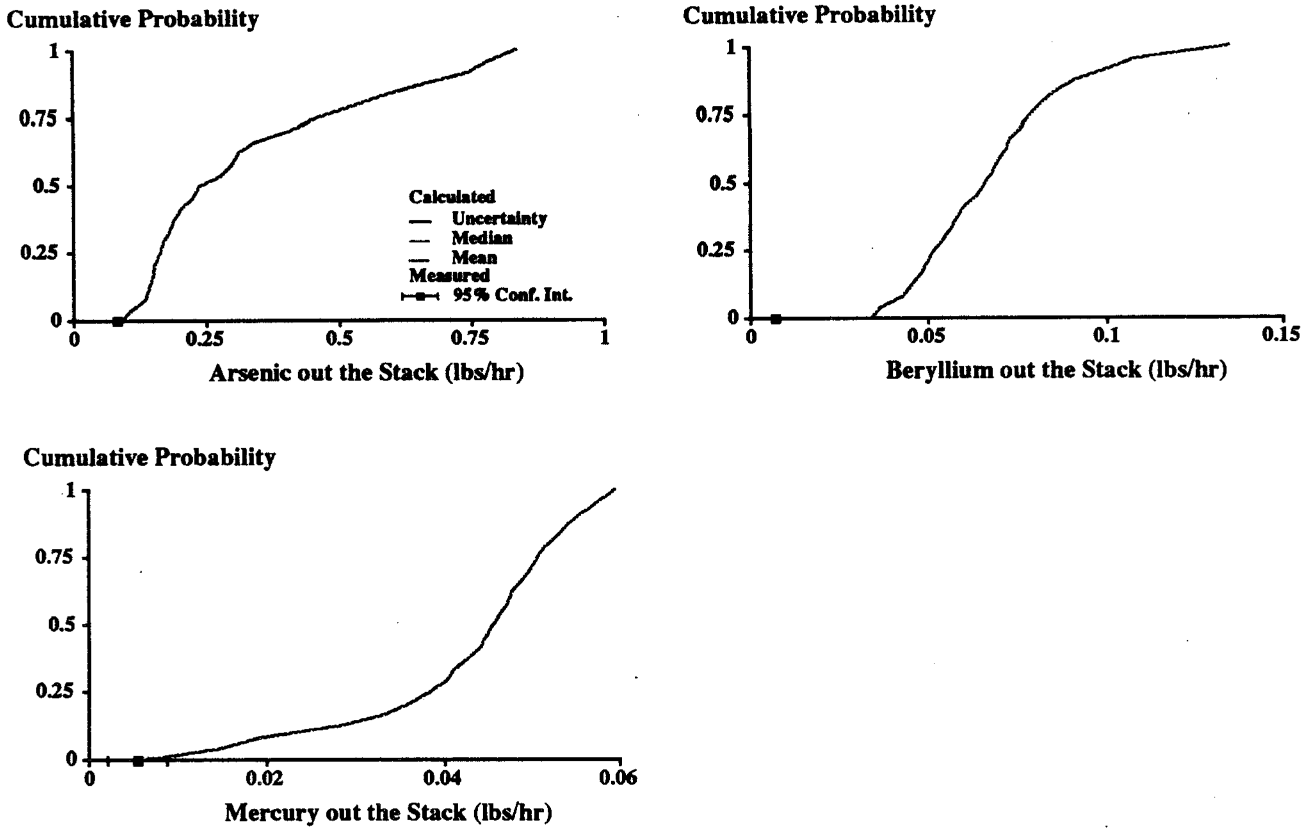


Figure 3. Stack emissions for Case I showing no overlap. Measured ranges are based on a normal distribution. Calculated curves are based on fractile distributions of coal measurements and PISCES database partition factors.

species for which there is reasonable or good agreement between measured and calculated emissions. In all six cases, the measured values falls within the range of calculated values. In five of these cases, the measured value falls near the median of the calculated distributions. Figure 3 shows four additional species for which there is little or no overlap between the reported and estimated emissions for this plant.

Because both the site-specific data and the PISCES database include only a small number of data points for each species, the range of measured emissions in Figures 2 and 3 is probably narrower than a complete data set would reveal. Also, the assumed furnace partitioning for the three species discussed previously artificially shifts to the right the calculated uncertainty curves. Thus, the results for arsenic and selenium would likely overlap to some extent if measured furnace partition factors were available. However, the effect would be small due to the high volatilization of these species at furnace temperatures and a subsequent partition of near unity.

Many of the uncertainty graphs display a long tail. This is almost entirely due to the ESP partition factor. The long tail represents low efficiency removal of trace species for some plants in the ESP database. The plant analyzed in Case I, on the other hand, employs a high efficiency precipitator. Experimental error also plays an important role in comparisons of model estimates and data. Table 2, for example, shows the overall closure on the plant mass balance for this site. The relatively poor degree of closure for a number of species undoubtedly affects the ability to model these rigorously. On a similar note, the poor degree of mass closure around the boiler at this site affects the calculation of precipitator partition factors.

Case II: A Coal-fired Power Plant with FGD

This case study focuses on a modern U.S. power plant equipped with a cold-side ESP and a wet flue gas desulfurization (FGD) system for SO_2 removal. To compare these new measurements with predictions based on the literature database, the power plant computer model was exercised using inputs describing the basic power plant and coal characteristics shown earlier in Table 1. The coal analysis included three field test samples, which

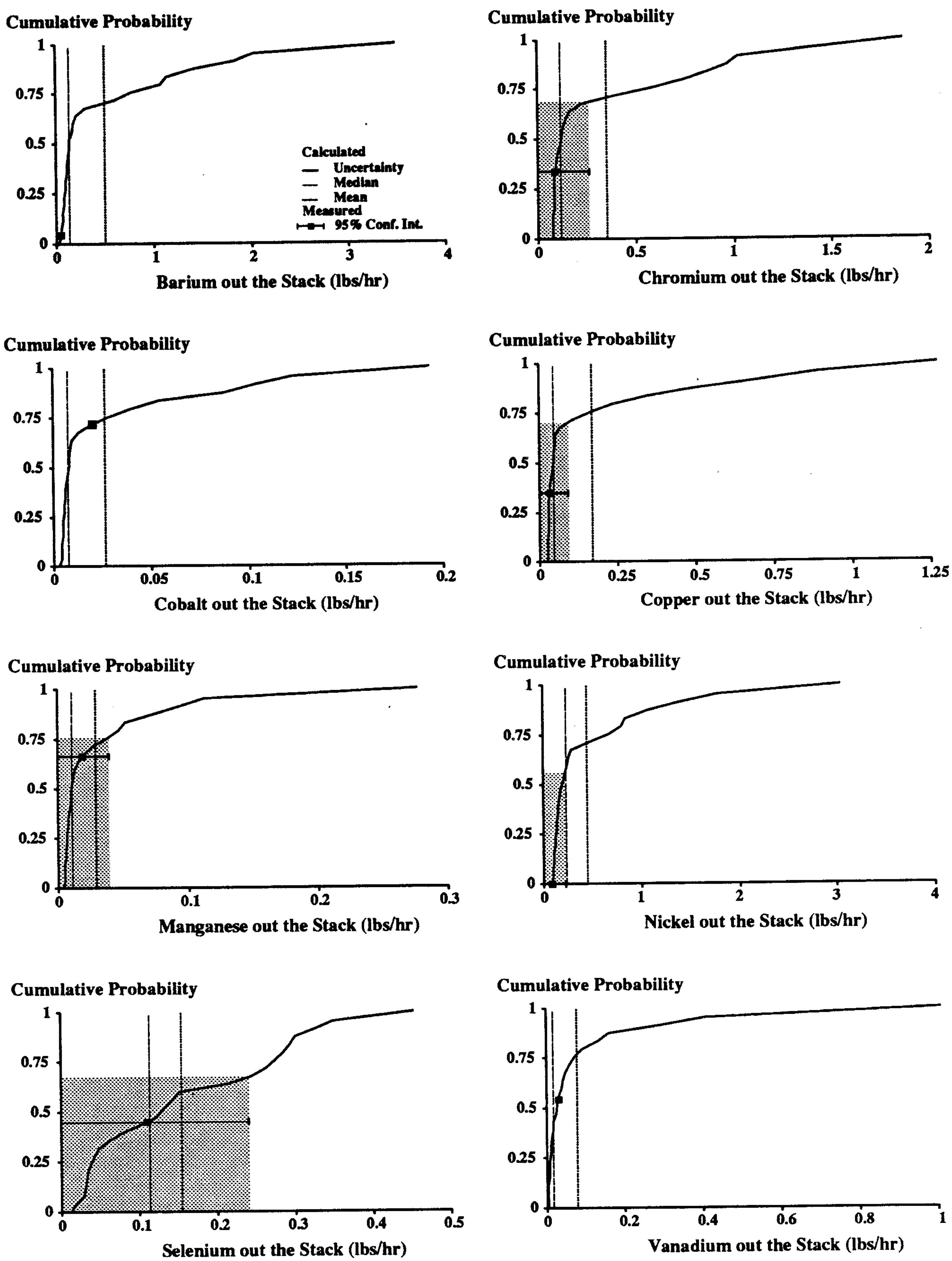


Figure 4. Stack emissions for Case II showing reasonable to good agreement. Measured ranges are based on a normal distribution. Calculated curves are based on fractile distributions of coal measurements and PISCES database partition factors. Regions of overlap are shown in gray.

were characterized probabilistically as in the previous case study. For this case, twelve trace species were modeled. All power plant parameters were treated deterministically using data provided by the host utility.

Plant Performance. The first set of comparisons between power plant data and model estimates focused on major plant flow rates including fuel input, flue gas flow rate, and solid waste streams. Excellent agreement (within a few percentages) was attained in all but two cases. For the flue gas flow rate exiting the stack, the initial difference between reported and predicted values was approximately 15 percent. However, upon further investigation it was discovered that the total excess air, including air preheater leakage, estimated by the power plant personnel differed from the value actually measured at the site. An analysis of excess oxygen levels at different points in the flue gas train revealed that inlet air leakage downstream of the boiler was much larger than had been believed. With the correct air leakage level specified, the model and field test data agreed well.

The other case of disagreement between modeled and measured values was the mass flow rate of FGD solids, where the reported value from the field testing was 20 percent below the value calculated based on the reagent stoichiometry and SO_2 removal efficiency reported for the power plant. Because no sulfur balance was performed as part of the field measurement plan, a definitive explanation for this difference is not available. However, the field test data implied a reagent stoichiometry much higher, and an SO_2 removal efficiency much lower than would be expected, suggesting that the sampled flow rate of FGD solids might have been in error.

Trace Performance. Turning to the trace species analysis, Table 2 reports the degree of closure between total mass input and total mass output for the trace species analyzed in this example. For five of the species the mass balance closure is within ±20 percent. For the remaining species the closure ranges from fair to poor (e.g., less than 50% closure for mercury). The measurement difficulties reflected by these data also influence any comparisons

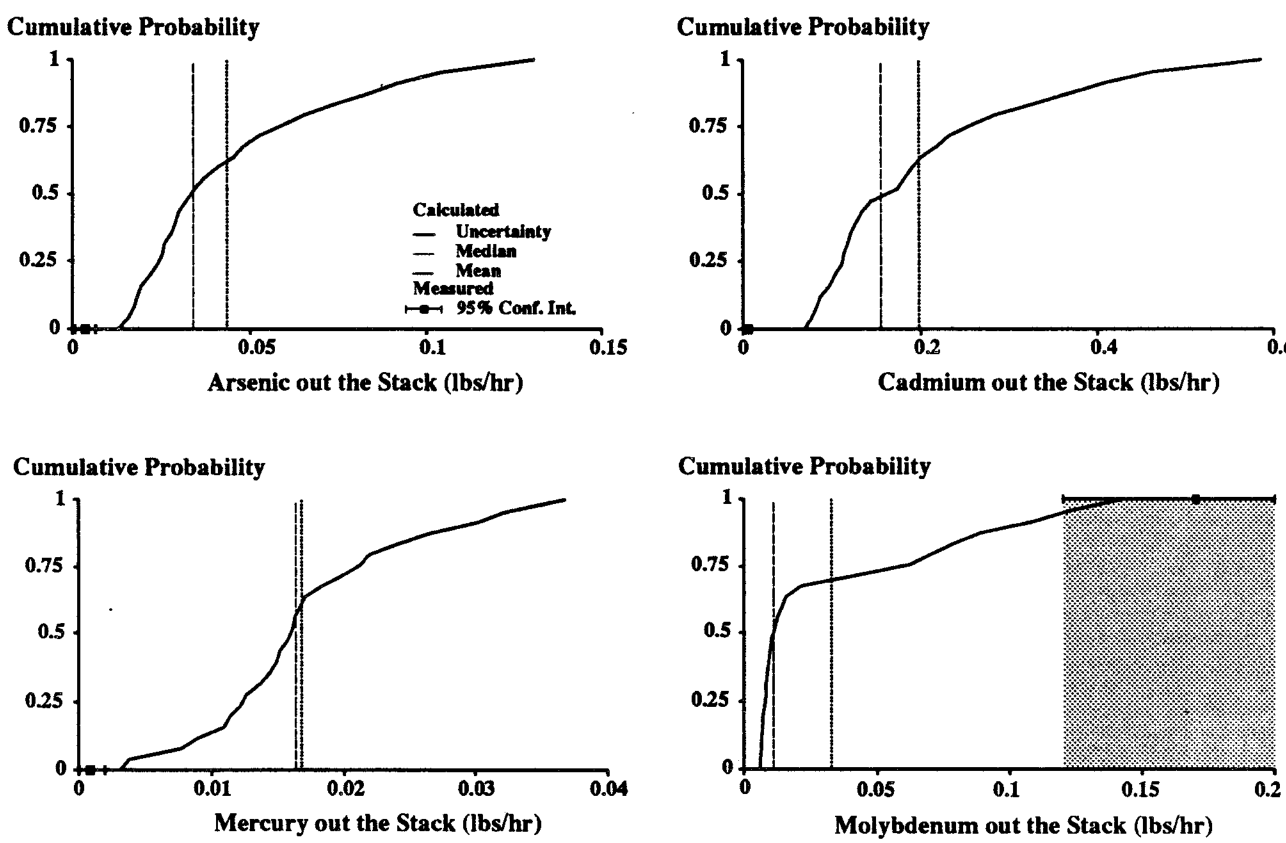


Figure 5. Stack emissions for Case II showing no overlap. Measured ranges are based on a normal distribution. Calculated curves are based on fractile distributions of coal measurements and PISCES database partition factors.

between data and model estimates.

Figures 4 and 5 present graphical comparisons between model predictions and field test data for this site. In these comparisons, the uncertainty in model estimates is due to the range of partition factor estimates from the PISCES database and the range of measured trace species concentrations for the coal actually burned. The partition factor estimates from the literature database typically are skewed, resulting in the positively skewed distributions for stack emissions rates predicted by the model. These calculated distributions indicate that there is a small probability of a high mass emission rate. Furthermore, because of the skewness of the distributions, the mean (average) values typically are higher than the median (50th percentile) values. For the stack emissions measurements from field test data for this particular site, an error bar reflects the 95 percent confidence interval reported for the trace species measurements.

Analysis. Figure 4 shows the eight species for which there is reasonable to good agreement between the predicted and measured values when the uncertainty in both of these estimates is considered. Nearly all of the species measurements are near or overlap with the median values of the calculated distributions. Figure 5 shows four additional species for which there is no overlap between measured and modeled estimates. For three of these four species the experimental mass balance was either poor or not determined.

The implication of Figure 4 is that in most cases the measured trace species emission rate is less than the value corresponding to the 70th percentile of the calculated cdf based on the current PISCES database. Figure 5 reminds us, however, that there are still exceptions that require further study. Indeed, for many of the trace species there are only a small number of available data points in the PISCES database to characterize uncertainty; in some case (e.g., FGD systems) only single point estimates are available. Thus, the current database does not likely reflect the full range of uncertainty in trace species behavior, underscoring the need for additional data acquisition.

The results from Case I and II should not be compared, because they are based on two different coals.

DISCUSSION

There are a number of challenges in analyzing trace species data. One involves understanding the difference between process variability and measurement error. Another involves dealing with correlation between distributions. A third involves approaches to dealing with data below the detection limit.

The data in the literature database as well as the field measurements represent some combination of process variability and measurement error. Process variability is the real difference in trace species concentration and partitioning as a function of time, depending for example on coal characteristics and process operating conditions. Furthermore, there may be variability from one plant to another in a larger population of plants of similar design, such as reflected in the PISCES database. Measurement error may have two components. One is a random error. The other is a systematic error or bias. In reality, process variability, random error, and systematic error may exist simultaneously in the measurements comprising both the literature database and the field test program. While systematic error is often the most difficult source of measurement error to quantify, the mass balance closures provide some quantitative indication of the magnitude of the error. Ideally, any measurement should be based on a validated test method for which there is prior information on both the random and systematic error. Unfortunately, because of the expense of taking measurements and of doing the analytical chemistry work, there is little information available for this purpose.

Understanding the difference between measurement errors and process variability would provide insight into the real sources of uncertainty in making model predictions. If uncertainty is due primarily to measurement errors, then uncertainty could be reduced by taking more (or larger) measurements or by developing better measurement techniques. If uncertainty is due primarily to process variability, either within a plant or across a population of plants of similar design, then uncertainty could be reduced by developing a better understanding of the effect of process conditions and environmental control equipment performance on trace species emissions, through parametric testing.

The source of uncertainty also has implications for estimating partitioning factors. Partitioning factors are typically based on measurements of inlet and outlet streams for a device. If measurement errors dominate, and if they are independent from one sample to another, then the estimates of partition factors would generally be highly uncertain. On the other hand, if process variability dominates, then partitioning factors could be estimated with a high degree of certainty assuming that process operating conditions are maintained constant throughout a test. In reality, this is very difficult to do at least in part because it is difficult to take simultaneous measurements at both the inlet and outlet of a device. Furthermore, it may be necessary to take measurements at several process conditions to either determine that certain partition factors are insensitive to operating conditions, or to characterize the effect of process conditions on trace species partitioning.

With regard to measurements below the detection limit, there are several possible courses of action. First and foremost is to ascertain whether the detection limit of the measurement technique is high enough to warrant regulatory concern. If a substance is not of regulatory or health concern at its detection limit, then it is unnecessary to pursue further analyses. However, in cases when an actual value below the detection limit still merits attention, Helsel [6] discusses several alternative approaches. Ultimately, judgment is required regarding the shape of the probability distribution of the quantity being measured. In essence, probability distributions can be extrapolated below the detection limit in cases where some data are available above the detection limit. In cases where all data are below the detection limit, judgment is required to make any characterization of uncertainty. While the use of judgment is often greeted with controversy, it is in fact the only practical way to deal with uncertainty given a lack of data. There are a number of techniques for dealing with expert judgments which enable the generation of insights into data needs and research priorities [7].

CONCLUSIONS

The two case studies described in this paper show that the power plant chemical assessment model developed as part of EPRI's air toxics program can be a valuable aide in estimating trace species emissions from coal-fired power plants, but that substantial uncertainty still exists in trace species emission estimates. Thus, single deterministic "emission factors" can give extremely misleading estimates of trace species emissions. Rather, probabilistic estimates of the type reported in this paper appear to be much more robust in representing the wide range of values that are observed.

The case study comparisons also underscore the importance of continued data acquisition and analysis. Various types of experimental errors and uncertainties appear to contribute significantly to the overall uncertainty in current emissions estimates, as does the variability in plant and fuel characteristics. The examples shown in this paper illustrate how the mass balance capabilities of the power plant assessment model can help identify inconsistencies in experimental data that can help in the interpretation and design of field sampling programs to obtain a better understanding of trace species emissions and their control. As part of future measurement activities, it is recommended that there be more attention to the notion of characterizing and separating process variability and measurement error.

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