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CHEMICAL CHARACTERIZATION OF POWER PLANT WASTE STREAMS

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INTRODUCTION

A key issue in the utilization of waste streams from conventional and advanced coal technology is the chemical characterization of such wastes or by-products. Traditionally, power plant stream compositions are characterized based on data from existing facilities and pilot plants. Depending on the by-product application or waste disposal method of interest, various physical properties of the waste also may be of interest. To an increasing extent, concern over the emissions and disposition of potentially hazardous or toxic chemical species also is becoming another important factor in the management of utility wastes.

This paper describes and illustrates a new computer model being developed for the Electric Power Research Institute (EPRI) to help characterize chemical emissions from conventional and advanced fossil fuel technologies. A new feature incorporated in this model is the ability to explicitly represent uncertainty in probabilistic terms, in contrast to conventional deterministic analysis. Development of this model has been stimulated primarily by the desire to better understand and quantify power plant design and operating factors that contribute to emissions of chemicals which may be regarded as potentially hazardous or toxic. However, one important application of this model will be the ability to characterize the chemical composition of utility waste streams including flyash, bottom ash, scrubber sludge, low volume liquid wastes, coal cleaning refuse, and other streams of interest to utility operators. In this paper, we briefly review the status design and implementation of this model, and illustrate how it can be used in conjunction with a chemical substances database to characterize waste or by-product stream constituents. Plans for future development also are summarized.

OVERVIEW OF MODEL STRUCTURE

The power plant chemical characterization model is designed to allow a user to easily configure a power plant for analysis, and to examine the implication of alternative design configurations, fuel choices and environmental control systems on the chemical composition of plant waste or by-product streams. The model uses a software system designed to provide flexibility in configuring different plant designs, and in analyzing results and associated uncertainties. The model currently operates on a MacIntosh-II computer. Software also is being designed to make the model accessible from other types of personal computers currently in use.

At its current stage of development, operation of the model requires knowledge of the underlying computer command language, much like any other model, spreadsheet program, database management system, or other computer-based applications. To bypass the need for mastering a new computer command language (which often is a major barrier or impediment to model use), efforts recently have been initiated to develop a truly user-friendly interface based on advanced graphical software capabilities which are now available. Figure 1 shows examples of several prototype computer screens which have been developed to demonstrate operation of the graphical interface. These screens also are useful for summarizing the general operation and data requirements of the model, examples of which are presented elsewhere.[1]

The first step in operating the model is to configure the power plant of interest. Present capabilities include conventional coal-fired, oil-fired and gas-fired plants, with advanced power generation technologies to be added later. Coal-fired plant configurations may be modeled in conjunction with various levels of coal cleaning as a means of altering the chemical composition and associated by-product or waste streams at the power plant. Table I lists the environmental control systems that currently can be selected in configuring a given power plant. (Additional environmental control technologies plus economic cost models will be added as part of on-going work.) Figures 1(a), (b) and (c) depict illustrative computer screens that will allow options to be selected simply by clicking on a graphical "button."

The next step in running the model is to set the value for each model parameter, and to specify the distribution of values for all parameters that are uncertain. The major plant sub-sections for an example plant configuration are listed in Figure 1 (d). For a typical coal-fired power plant, the model contains approximately 100 user-specified parameters related to plant design and performance. Figure 1(e), for example, illustrates a computer input screen that may be used to specify several parameters for the boiler/steam cycle subsystem of the overall power plant. Default parameters are provided for many of the parameters of each plant section, though these defaults easily may be overridden.

Probabilistic Analysis Capability

As noted earlier, a unique capability of the power plant chemical characterization model is that it can perform probabilistic analysis using Monte Carlo simulation methods. To specify the uncertainty in any input parameter, the user may choose from a number of standard probability distributions (e.g., normal, lognormal, uniform, triangular, chance and others), as illustrated in Figure 1(f). Alternatively, any arbitrary distribution may be specified in continuous or discreet form. To carry out a probabilistic analysis, the user then chooses one of three sampling methods (typically random Latin Hypercube sampling) and the number of iterations or sample size. There is also provision for treating correlated input variables.

TABLE I Current technology options in power plant model.

Fuel Characteristics
- Coal
- Oil
- Gas

Boiler Parameters
- Tangential
- Wall
- Cyclone

NOx Controls
- Low NOx Burners

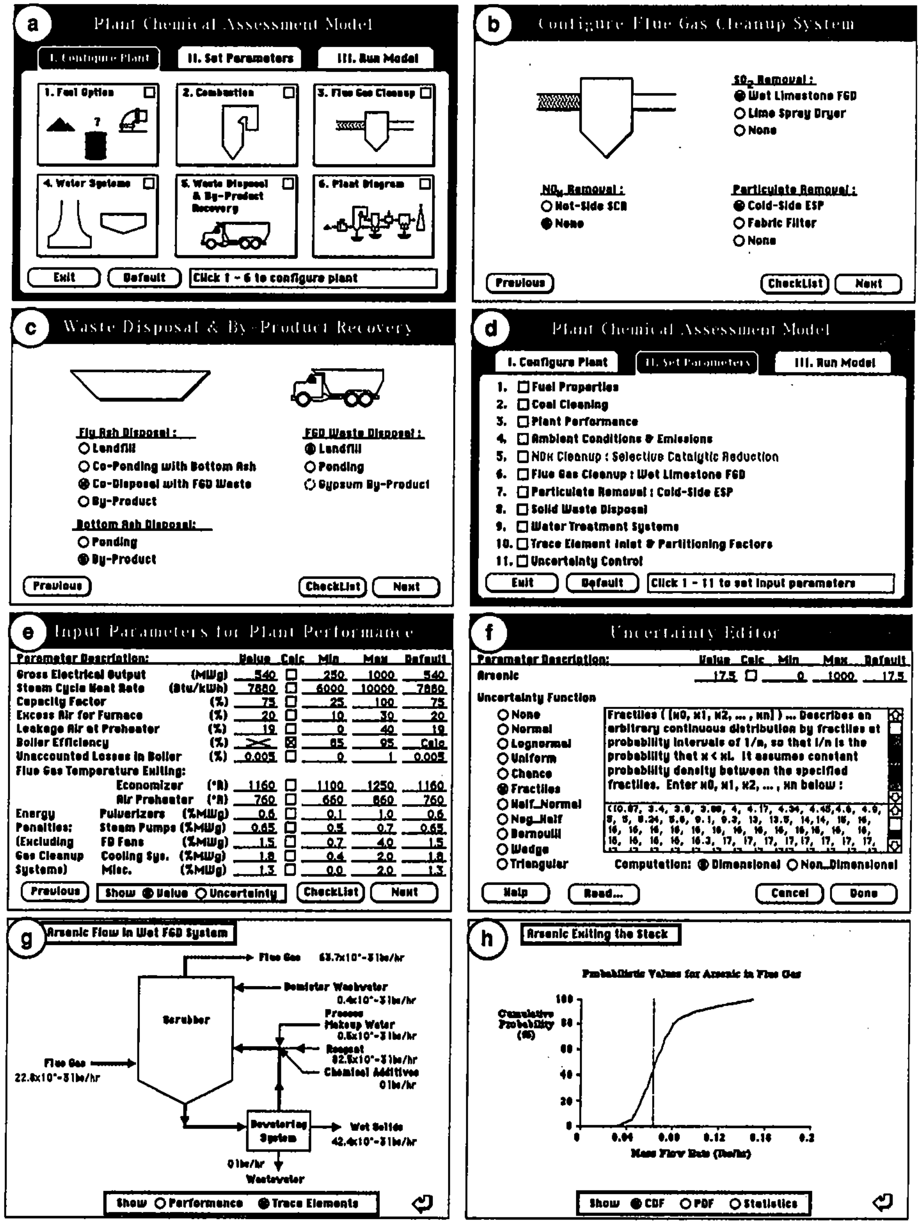
Particulate Controls
- Precipitator
- Fabric Filter

SO2 Controls
- Wet Lime FGD
- Wet Limestone
- Lime Spray Dryer

Solid Waste Disposal
- Landfill
- Ponding
- Co-Disposal

Cooling Water System
- Once-Through
- Cooling Tower
- Pond or Lake
- Fresh or Saline

Water Treatment Systems
- Plant Makeup Water
- Plant Service Water
- Boiler Makeup
- Condensate Polisher
- Cooling Tower Makeup
- Tower Slip Stream
- Ash Pond Discharge



b SO$_2$ Removal:
- ● Wet Limestone FGD
- ○ Lime Spray Dryer
- ○ None

NO$_x$ Removal:
- ○ Hot-Side SCR
- ● None

Particulate Removal:
- ● Cold-Side ESP
- ○ Fabric Filter
- ○ None

c Fly Ash Disposal:
- ○ Landfill
- ○ Co-Ponding with Bottom Ash
- ● Co-Disposal with FGD Waste
- ○ By-Product

Bottom Ash Disposal:
- ○ Ponding
- ● By-Product

FGD Waste Disposal:
- ● Landfill
- ○ Ponding
- ○ Gypsum By-Product

d
1. ☐ Fuel Properties
2. ☐ Coal Cleaning
3. ☐ Plant Performance
4. ☐ Ambient Conditions & Emissions
5. ☐ NOx Cleanup : Selective Catalytic Reduction
6. ☐ Flue Gas Cleanup : Wet Limestone FGD
7. ☐ Particulate Removal : Cold-Side ESP
8. ☐ Solid Waste Disposal
9. ☐ Water Treatment Systems
10. ☐ Trace Element Inlet & Partitioning Factors
11. ☐ Uncertainty Control

e

Parameter Description:			Value	Calc	Min	Max	Default
Gross Electrical Output		(MWg)	540	☐	250	1000	540
Steam Cycle Heat Rate		(Btu/kWh)	7880	☐	6000	10000	7880
Capacity Factor		(%)	75	☐	25	100	75
Excess Air for Furnace		(%)	20	☐	10	30	20
Leakage Air at Preheater		(%)	19	☐	0	40	19
Boiler Efficiency		(%)	><	☒	85	95	Calc
Unaccounted Losses in Boiler		(%)	0.005	☐	0	1	0.005
Flue Gas Temperature Exiting:							
	Economizer	(°R)	1160	☐	1100	1250	1160
	Air Preheater	(°R)	760	☐	660	860	760
Energy	Pulverizers	(%MWg)	0.6	☐	0.1	1.0	0.6
Penalties:	Steam Pumps	(%MWg)	0.65	☐	0.5	0.7	0.65
(Excluding	FD Fans	(%MWg)	1.5	☐	0.7	4.0	1.5
Gas Cleanup	Cooling Sys.	(%MWg)	1.8	☐	0.4	2.0	1.8
Systems)	Misc.	(%MWg)	1.3	☐	0.0	2.0	1.3

Show ● Value ○ Uncertainty

f

Parameter Description:	Value	Calc	Min	Max	Default
Arsenic	17.5	☐	0	1000	17.5

Uncertainty Function
- ○ None
- ○ Normal
- ○ Lognormal
- ○ Uniform
- ○ Chance
- ● Fractiles
- ○ Half_Normal
- ○ Neg_Half
- ○ Bernoulli
- ○ Wedge
- ○ Triangular

Fractiles ([x0, x1, x2, ... , xn]) ... Describes an arbitrary continuous distribution by fractiles at probability intervals of 1/n, so that i/n is the probability that x < xi. It assumes constant probability density between the specified fractiles. Enter x0, x1, x2, ... , xn below :

{0.07, 3.4, 3.8, 3.88, 4, 4.17, 4.34, 4.45,4.6, 4.9, 5, 5, 5.24, 5.6, 9.1, 9.3, 13, 13.5, 14,14, 16, 16, 16, 16, 16, 16, 16, 16, 16, 16, 16,16, 16, 16, 16, 16, 16, 16, 16, 16.3, 17, 17, 17, 17,17, 17, 17, 17,

Computation: ● Dimensional ○ Non_Dimensional

g Show ○ Performance ● Trace Elements

h Show ● CDF ○ PDF ○ Statistics

Figure 1: Sample Screens for the Graphical Model Interface

Once the power plant configuration has been established and all parameter values have been set, the model is ready to run. Using mass and energy balance relationships, together with empirical data where necessary, the mass flow rates of all gaseous liquid and solid streams entering and exiting the plant are computed, and the chemical composition of each stream determined. Where input parameters have been specified probabilistically, the resulting uncertainty induced in output stream quantities is reported in terms of a probability distribution showing the likelihood of different results. This analytical capability is important to a number of potential model applications, including the chemical characterization of potential by-products or plant waste streams. Figures 1(g) and (h) illustrate the types of deterministic and probabilistic results that will be available using the graphical user interface.

Interface with the Chemical Database

Probabilistic analysis is particularly useful in characterizing the quantities of trace chemical constituents likely to be present in various plant waste streams or by-products. To carry out such an analysis, uncertainties must be specified for, (1) the quantities of trace constituents entering the plant in fuel, reagents, water and air, and (2) the "partitioning" fractions of plant components or removal efficiency capabilities of various environmental control systems. To characterize the quantities of trace species formed as a result of physical or chemical reactions within the power plant (e.g., trace organic compounds and certain metallic wastes), empirical data must be used in lieu of a first principles analysis based on mass and energy conservation. The auxiliary input data needed to characterize trace species input streams and the performance of environmental control technologies and plant subsystems currently is being assembled by Radian Corporation in a companion project (known as PISCES, for Powerplant Integrated Systems: Chemical Emissions Studies) sponsored by EPRI.[2] When completed, this database will contain systematic information on all chemical species of interest to the electric utility industry for both conventional and advanced power generating systems. Other information of interest (e.g., measurement methods, regulatory limits, etc.) also is included in the database. An automated interface between the chemical substances database and the power systems emissions model also is being developed to facilitate future analyses.

AN ILLUSTRATIVE CASE STUDY

The capabilities of the probabilistic computer model to characterize trace constituents in power plant by-products or waste streams is illustrated here for the simple case of a coal-fired power plant with an electrostatic precipitator (ESP) and no SO_2 removal system. This configuration is one of ten plant designs selected by Radian and Bechtel Corporations to represent typical U.S. power plant installations. Nominal stream flow rates calculated from the Carnegie Mellon computer model for these configurations were verified by independent calculations performed by Bechtel as part of the EPRI PISCES project. All plant designs are for a nominal 350 MW (net output) system. Table II lists some of the input assumptions regarding plant design and fuel characteristics.

The case study presented here focuses on a quantification of two trace elements (arsenic and chromium) in the collected flyash stream. The PISCES database was used to estimate the distribution of trace elements in coal, and the partitioning of each species in the boiler and electrostatic precipitator. Figure 2 shows a histogram of the coal concentration data used for the analysis. These data, which show more than a tenfold range in concentration, reflect the distributions of arsenic and chromium in eastern bituminous coals. These frequency distributions, quantified into fractiles, were part of the input to the model. Similarly, distribution functions were used to quantify the fractions of arsenic and chromium reporting to the bottom ash and flyash streams, and the fractions removed by the ESP, according to the current database. In this analysis, uncertainties also were assigned to several plant design and operating parameters, as indicated in Table III.

Figures 3 and 4 summarize results of the analysis in terms of a frequency distribution showing the annual mass flow rates of arsenic and chromium in the bottom ash and flyash collected from this hypothetical 350 MW plant. These results also show the contribution of uncertainty in power plant factors alone (especially the partitioning of elements to the bottom ash and flyash). Note that the overall distribution is sharply skewed relative to the expected (deterministic) values obtained using only the nominal or values of all input parameters. For arsenic in flyash, for example, the 90 percent confidence interval (reflecting the range between probabilities of 5 and 95 percent) ranges from 0.1 to 16.6 tons/yr in total emissions, with a median value of 2.7 tons/yr. Figure 5 shows similar results for arsenic and chromium mass concentration in collected flyash. For chromium, for example, the 90 percent confidence interval ranges from approximately 10 to 500 parts per million, with a median value of 111 ppm. In this example, a large part of the total uncertainty arises from uncertainty in trace metal coal concentrations, which reflect composite data for a collection of eastern bituminous coals. For any one coal, however, a tighter confidence band would be expected.

CONCLUSION

These results illustrate the types of chemical characterization analyses that will be possible using a new probabilistic chemical assessment model and power systems

TABLE II Selected model input assumptions for illustrative case study.

Power System Parameters	
Boiler Firing Type	Tang.
Gross Electrical Capacity, MW	383.7
Steam Heat Rate, Btu/kWh	7872
Boiler Efficiency, %*	89.1
Capacity Factor, %	65
Excess Air to Boiler, %	17.9
Excess Air Leakage, %	12.2
Economizer Temperature, °F	740
Air Pre-Heater Temperature, °F	277
Auxiliary Power Requirements, %MW	
Pulverizer	0.6
Steam Pump	0.65
Particulate Collector *	0.18
Total Fans	1.5
Solid Waste Disposal *	0.0
Cooling Water System	0.4
Miscellaneous Elect	1.3
Coal Composition	
Name	Illinois #6
Mine/Location	Illinois
HHV, Btu/lb	11,241
Carbon, wt %	61.19
Hydrogen, wt %	4.69
Oxygen, wt %	8.82
Sulfur, wt %	3.40
Nitrogen, wt %	1.10
Moisture, wt %	12.0
Ash, wt %	8.80
Air Properties and Emission Limits	
Ambient Temperature, °F	80
Ambient Pressure, psia	14.687
Humidity, lb H_2O/lb dry air	0.0063
NOx Emissions, lb NO_x/ton coal	14.14
NO/NO_2 Molar Ratio	95/5
SO_2/SO_3 Molar Ratio	97/3
Overhead Ash, wt %	75
Sulfur in Bottom Ash, wt %	2.5
Carbon in Ash, wt %	0
Carbon to CO, Molar %	0
Particulate Limit, lb/MBtu	0.03
NOx Limit, lb/MBtu	0.6
Effluent Discharge Limits	NPDES
Particulate Collector	
Removal Efficiency, % *	99.5
Once Through Cooling Water System	
Auxiliary Cooling, % heat load	1.4
Temperature Range, °F	37
Solid Waste Disposal	
Sluicing Water Evaporated, lb/lb ash	0.75
Solids in Bottom Ash, wt %	73.9
Solids in Ash Pond, wt %	85
Solids in Fly Ash, wt %	100

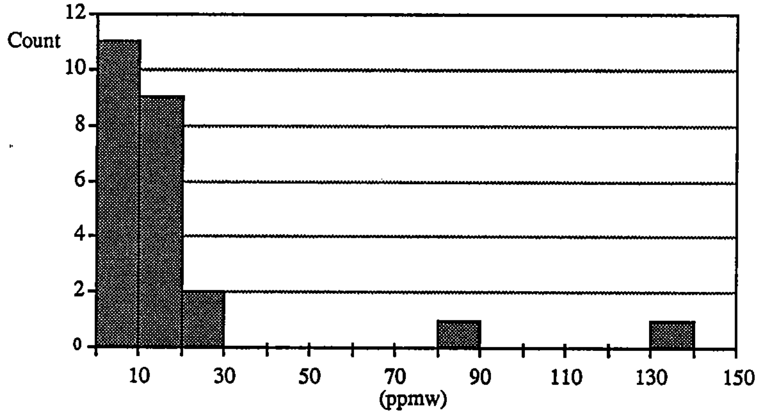
* Can either be calculated or entered as an input parameter.

TABLE III selected uncertainty assumptions for illustrative case study.

Parameter	Nominal Value	Uncertainty Distribution
Power System Parameters		
Steam Heat Rate, Btu/kWh	7872	Negative Half Normal ($\sigma = 1.8\%$)
Capacity Factor, %	65	Triangular (50, 65, 75)
Excess Air Boiler, %	17.9	Normal ($\sigma = 2.5\%$)
Total Air Leakage, %	12.2	Normal ($\sigma = 2.5\%$)
Auxiliary Power Requirements		
Particulate Collector, %	0.18	Normal ($\sigma = 10\%$)
Air Properties and Emission Limits		
Overhead Ash, wt %	75	Fractiles (68.7, 69.4, 73.0, 75.5)
Trace Species Parameters[a]		
Arsenic Concentration in Coal	10.5	Fractiles
Chromium Concentration in Coal	12.6	Fractiles
Ar Conc. Ratio, Bottom to Total Ash	0.21	Fractiles
Cr Conc. Ratio, Bottom to Total Ash	0.81	Fractiles
Removal Efficiency of Ar in ESP	0.953	Fractiles
Removal Efficiency of Cr in ESP	0.998	Fractiles

[a] Fractiles obtained from PISCES database used as model input.

(a) Arsenic Concentration in Coal



(b) Chromium Concentration in Coal

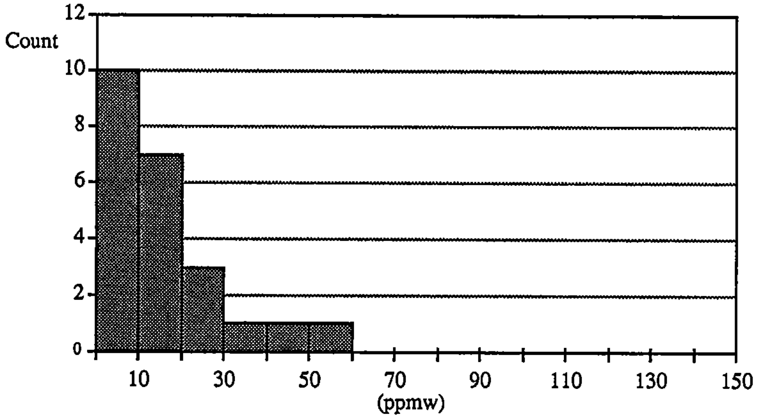
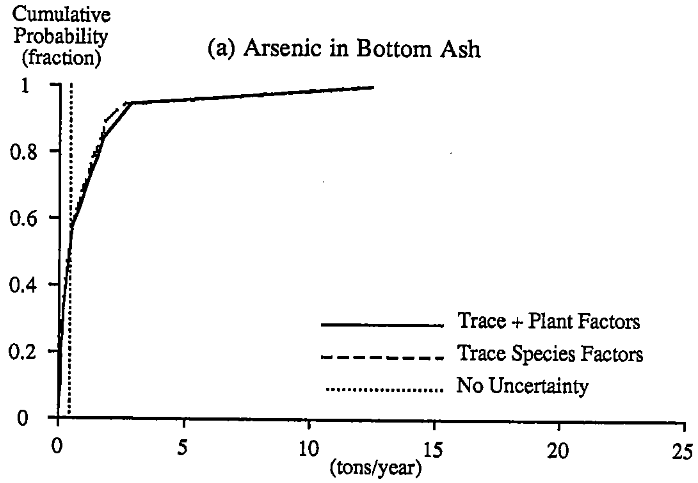


FIGURE 2 **Model input data for trace element distributions in coal.**

(a) Arsenic in Bottom Ash



(b) Chromium in Bottom Ash

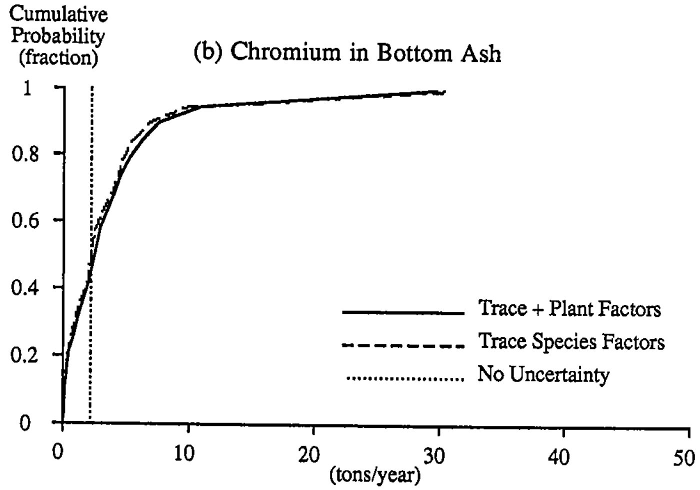


FIGURE 3 **Probabilistic results for bottom ash emissions rates.**

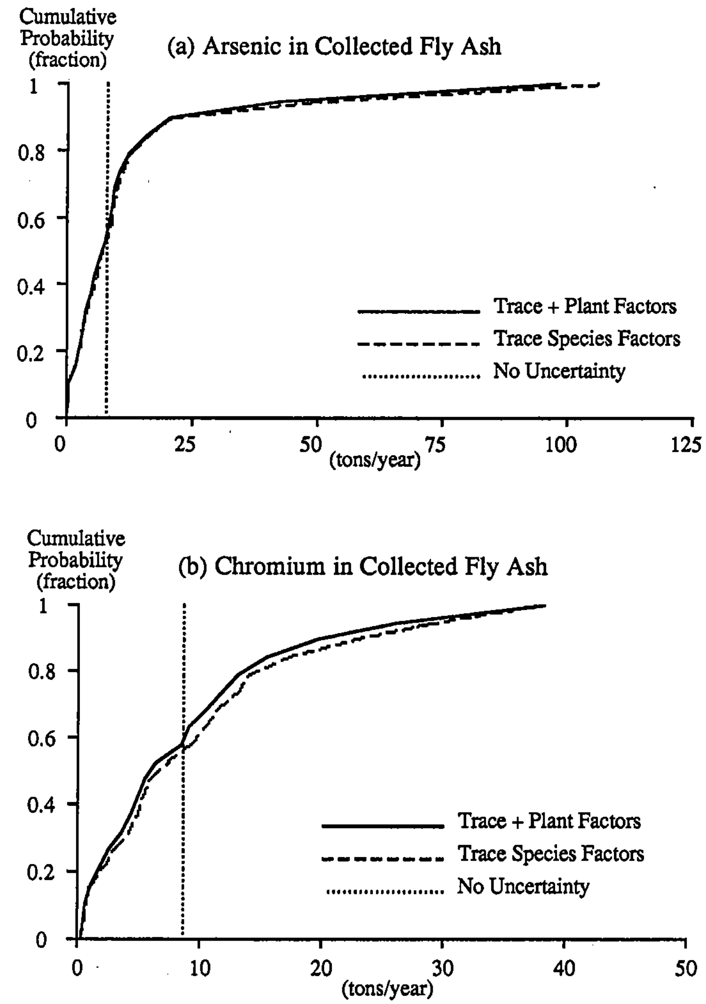


FIGURE 4 Probabilistic results for flyash emissions rates.

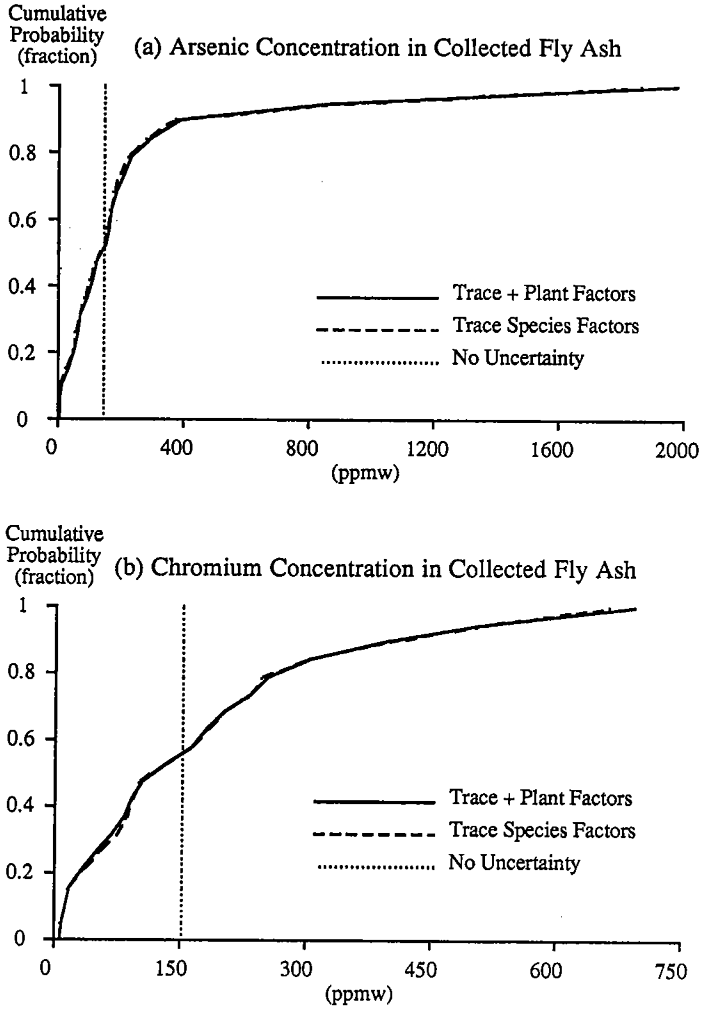


FIGURE 5 Probabilistic results for flyash concentrations.

chemical substances database now under development for EPRI. Version 1.0 of the model is expected to be completed and transferred to EPRI early in 1991. Current efforts are focused on model validation, development of the user-friendly interface, and development of an interface with the PISCES database. Subsequent work also will include the incorporation of economic cost models and expansion of the technology set to include a number of advanced power generation options including fluidized bed combustion, integrated gasification combined cycle systems, refuse-derived fuels, and other new technologies. Continuous updating of the chemical substances database is expected to proceed in parallel with new model developments to facilitate the chemical characterization of power plant waste streams.

ACKNOWLEDGMENTS

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