ABSTRACT

CHEN, JIANJUN. Optimization of Cost and Emissions of a KRW-Gasifier based IGCC System under Variability and Uncertainty (Under the supervision of Dr. H.C. Frey).

Optimization of process technologies under uncertainty has been extensively studied in the literature. It provides a rigorous and powerful tool for the design of advanced technologies. Two methods are available for optimization of process models under uncertainty, which are stochastic optimization and stochastic programming. From the results of the two methods, Expected Value of Perfect Information (EVPI) can be estimated, which provides decision-makers the expected value of maximum benefit of reducing uncertainty. However, optimization of process models under uncertainty has not made distinctions between variability and uncertainty. Variability is a heterogeneity of values for a quantity over time, space or among different members of a population, while uncertainty is a lack of information. This study proposes two methodologies for optimization of process models when both variability and uncertainty in model parameters are considered. One is a coupled stochastic optimization and programming method, which involves stochastic optimization for each realization of variability and enables one to evaluate the effect of uncertainty on optimal designs. The other one is a two-dimensional stochastic programming technique, which features stochastic programming for each realization of variability and produces two-dimensional distributions of deterministic optimal solutions. Comparing the outputs of the two methods, both point estimates and confidence intervals of EVPI can be estimated. The two methods are demonstrated through application to optimization of the cost and emissions of a KRW-Gasifer based IGCC system when both variability and uncertainty in model parameters are considered.

The methodologies proposed and demonstrated in this study are helpful to design and evaluation of advanced technology applications where cost minimization, risk analysis, environmental compliance and R&D priority remain important issue.

Keywords: Variability, Uncertainty, Stochastic Optimization, Stochastic Programming, Expected Value of Perfect Information (EVPI), IGCC.

OPTIMIZATION OF COST AND EMISSIONS OF A KRW-GASIFIER BASED IGCC SYSTEM UNDER VARIABILITY AND UNCERTAINTY

by

JIANJUN CHEN

A thesis submitted to the Graduate Faculty of
North Carolina State University
in partial fulfillment of the
requirements for the Degree of
Master of Science

DEPARTMENT OF CIVIL, CONSTRUCTION AND ENVIRONMENTAL ENGINEERING

Raleigh

2003

APPROVED BY

Chair of Advisory Committee

BIOGRAPHY

Jianjun Chen got his Bachelor's degree from Environmental Science and Engineering Department at Tsinghua University, China in 2001. There, he studied mobile source related air pollution problems under the guidance of Professor Lixin Fu. Upon graduation, he came to North Carolina State University for his Master's degree in Environmental Engineering. He was a research assistant in Dr. Frey's group, and worked on vehicle emissions modeling and optimization of process models. After receiving his Master's degree, he will attend University of New Hampshire for his Ph.D.'s degree. His research will be concerned with atmospheric aerosols and air quality models.

ACKNOWLEDGEMENT

First of all, I want to thank Dr. Frey, my advisor, for providing me with a research assistantship. Study under Dr. Frey's guidance was stimulating and also joyful. I am particularly excited about being given chance to work on modeling vehicle emissions. Meanwhile, I take this opportunity to thank Dr. Frey's support and patience during my long vacation at China (Due to visa problem). I would also like to express my thanks to other two committee members: Dr. Ranjithan and Dr. Brill for their time and helps.

I want to extend my appreciation to other people in Dr. Frey's research group. They are: Allen, Alper, Amir, Kaishan, Maggie, Minsheng, Yunhua, and Tanwir. Particularly, to Allen for going through my thesis again and again; to Alper for sharing me with his knowledge and experiences in vehicle emissions; to Kaishan for many helps which made it possible that I can work partly at home when I was waiting for visa. Specially, I am indebted to Minsheng. My life here became much easier thanks to his kind and generous helps during the past two years.

I am grateful to my families: my father and mother, younger brother and others, for their love, support and sacrifice made to allow me keeping staying at schools (Unfortunately, I will spend probably another four years in school).

Lastly but not the least, I would like to thank many of my friends (middle and high school classmates, college classmates) for their continuous cares and support. Particularly, to Zhaoqing, our friendship will be life-long; to Xujuan, for the love that I will never forget.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

1.0 INTRODUCTION

The emphasis of environmental design for process technologies is shifting from one pollutant to multiple pollutants, and multiple environmental media. Properly integrated system models are needed to assess the complex interactions among many components of highly coupled system. For example, Frey and Rubin (1992a) developed integrated model for environmental control in integrated gasification combined cycle systems (IGCC); Rubin *et al*. (1997) developed integrated environmental control model for coal-fired power systems; Bharvirkar and Frey (1998) developed simplified performance, emissions and cost model for integrated gasification combined cycle systems (IGCC).

For all technologies in an early phase of development, there are always uncertainties in the performance and cost estimates (Frey and Rubin, 1991a). Chemical engineers and technical managers involved in research, development and demonstration (RD&D) of advanced process can benefit from a systematic approach for characterizing uncertainties in new process technologies (Frey and Rubin, 1992b). Uncertainty analysis has been applied to advanced SO_2/NO_X control technology (Frey and Rubin, 1991a), coal utilization and environmental control in integrated gasification combined cycle systems (Frey and Rubin, 1992; Frey, *et al*., 1994), integrated environmental control of coal-fired power systems (Rubin, *et al*., 1997). Uncertainties in model parameters were found to significantly affect the cost of the system (Frey and Rubin, 1991a; Frey and Rubin, 1992; Frey *et al*., 1994; Rubin *et al*., 1997).

For an integrated process system, there are always a wide variety of feed stocks, products and technologies, optimization is particularly critical for optimal design and for meeting with site-specific needs (Bjorge *et al*., 1996). For example, Diwekar *et al*. (1992)

optimized the SO_2 control in an IGCC system. George *et al*. (1992) optimized the cost of electricity for an IGCC power plant, and found that annual savings for optimized design can exceed 2.2 million (mid-1990) dollars.

Combined with uncertainty analysis, optimization methods provide a powerful and rigorous tool for design of process technologies. Diwekar *et al*. (1997) summarized and demonstrated two methods for optimization of process models under uncertainty. One is termed as stochastic optimization, which enables one to use statistics, such as expected value, variance and other statistics, as objective function values or as constraints. Another is termed as stochastic programming, which enables one to evaluate the sensitivity of optimal solutions to uncertainty in model parameters. Stochastic optimization and programming techniques can ensure that during design phases, issues such as cost minimization, risk analysis, environmental compliance and R&D prioritization, can be fully and rigorously considered (Diwekar *et al*., 1997). Stochastic optimization has been applied by many researchers (Dantus and High, 1999, Hou *et al*., 2000; Kim and Diwekar, 2002a, 2002b). Application of stochastic programming to process models has not become popular, perhaps mostly because of its computational intensity and lack of easy-to-use software tools, although sensitivity of optimal solutions to model parameters has been studied by some researchers (Cocks *et al*., 1998; Jack and Tybirk, 1998; Pinto, 1998; Fournier, *et al*., 1999).

Uncertainty analysis or optimization under uncertainty for process technologies has not made distinctions between variability and uncertainty. Variability is a heterogeneity of values for a quantity over time, space or among different members of a population (Zheng, 2002), while uncertainty is a lack of information. Distinction between uncertainty and variability has been gaining wide acceptance in risk assessment (NRC, 1994) and environmental pollutant inventory (Frey and Bammi, 2002, Frey and Zheng, 2002). Distinction between variability and uncertainty has rarely been done in probabilistic analysis or optimization of process technologies only until recently by Frey and Zhang (2003), Rooney and Biegler (2003). Rooney and Biegler consider two types of unknown input parameters, uncertainty model parameters, and variable process parameters. In the former case, a process is designed that is feasible over the entire domain of uncertain parameters, while in the later case, control variables can be adjusted during process operation to compensate for variable process parameters. However, their work does not address uncertainty in parameters that characterize variability in an input.

The objective of this study is to develop and demonstrate optimization of process technologies when both variability and uncertainty in model parameters are considered. Based on stochastic optimization and stochastic programming methods discussed by Diwekar, *et al*.(1997), two methods are proposed for doing optimization under both variability and uncertainty. One is termed as a coupled stochastic optimization and programming technique, which involves stochastic optimization for each realization of uncertainty. Another is termed as a two-dimensional stochastic programming technique from which two dimensional distributions of optimal solutions can be produced for evaluation of the effect of both variability and uncertainty on optimal solutions. The two methods are then applied to optimization for a KRW gasifier based IGCC system when variability and uncertainty in model parameters are considered.

This thesis is organized as follows:

Chapter 2 discusses the basic concepts of variability, uncertainty, stochastic optimization and stochastic programming. Based on these, optimization techniques under both variability and uncertainty are proposed.

Chapter 3 gives an overview for the Integrated Combined Cycle System (IGCC). In this study, a KRW gasifier based IGCC system is used as an example to demonstrate optimization techniques when variability and uncertainty in model parameters are considered. Variables with variability and/or uncertainty among IGCC model parameters are identified. Probabilistic distributions are developed for these variables.

Chapter 4 describes the random number generator and optimizer used in this study. AuvTool, which was developed by Zheng and Frey (2002), is used as random number generator. Evolver, a commercial Genetic Algorithm based optimization solver, is adopted as optimizer.

Chapter 5 presents the results of optimization of the IGCC system when variability and uncertainty in model parameters are considered.

Chapter 6 presents conclusions of this thesis, and recommendations for future studies.

2.0 CONCEPT AND METHODOLOGY

This chapter discusses basic concepts of variability and uncertainty, stochastic optimization and stochastic programming. Based on these, coupled stochastic optimization and programming technique, and two dimensional stochastic programming are proposed.

2.1 Variability and Uncertainty

Variability is a heterogeneity of a quantity over time, space or among different members of a population (Zheng, 2002). For example, in a complex coal gasification system, many parameters are subject to variations, such as physical and chemical properties of inlet materials; material conversion rate in the system and so on. Variability can be represented by frequency distributions showing the variation of the quantity (Frey, 1997).

Uncertainty refers to a lack of knowledge regarding the true value of a quantity. Draper et al. (1987) pointed out that there are three main sources of uncertainty in any problem:

(1) Uncertainty about the structure of a model;

(2) Uncertainty about the estimates of the model parameters, assuming that the structure of the model is known;

(3) Unexplained random variation in observed variables even the structure of the model and the values of the model parameters have been known.

Specifically, uncertainty in parameters can come from lack of data, non-representative of data, random sampling errors and measurement errors. Probability distributions can be employed to represent the likelihood that a quantity falls into a particular range (Cullen and Frey, 1999).

Distinction between variability and uncertainty can be important for policy and scientific reasons (Frey and Rhodes, 1998). In setting policy on control of emissions into environment, we may wish to protect the health of at least a given portion of the population and to do so within an acceptable confidence level. For example, we may wish to be 92% confident that we reduce the health risks of at least 96% of the population below some level. Knowledge regarding variability can be used to identify subgroup which should receive special consideration, while uncertainty can be used to prioritize additional research (Frey and Rhodes, 1998).

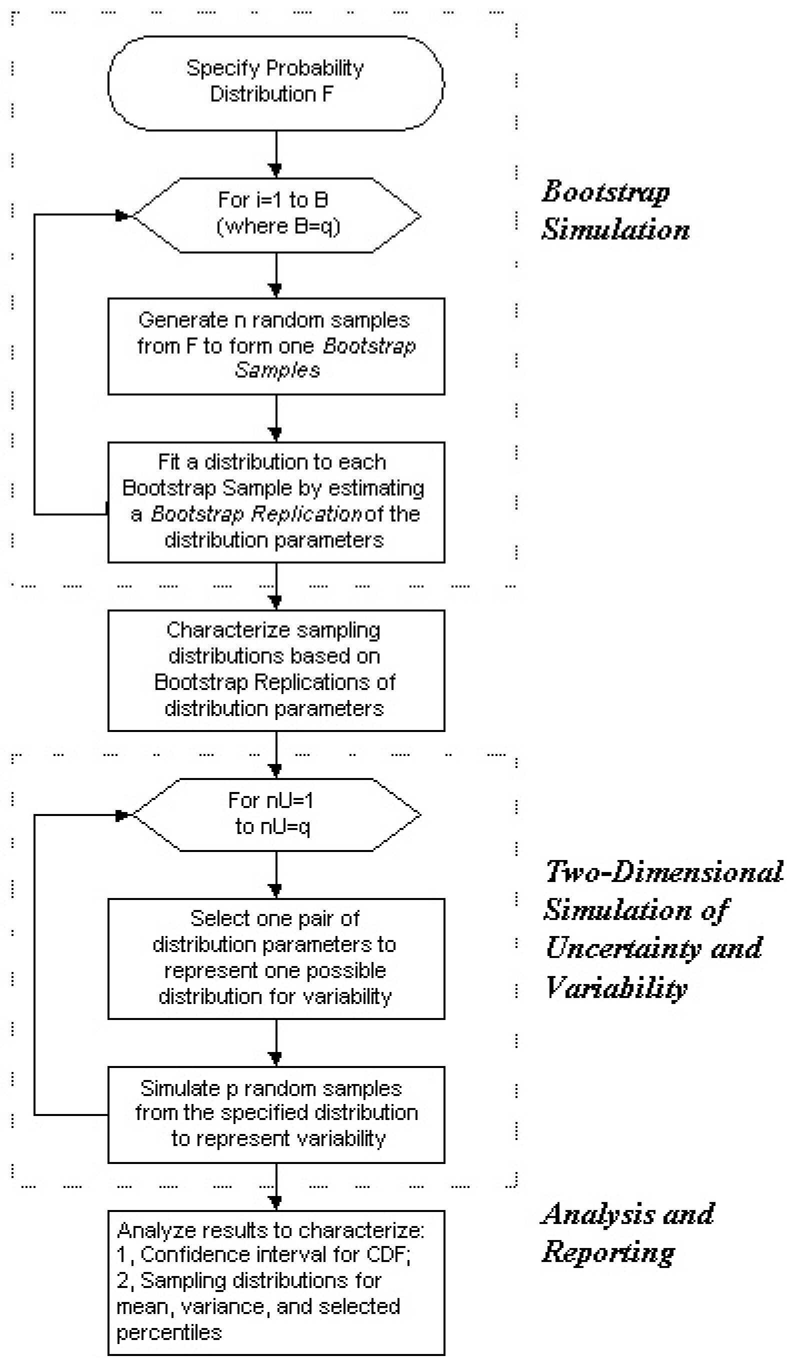
2.2 Sampling Technique for Variability and Uncertainty

As pointed out above, frequency distributions are used to characterize variability in a quantity, and probability distributions are used to represent uncertainty of a quantity. Numerical sampling techniques, such as Monte Carlo simulation or Latin hypercube sampling, can be employed to generate random numbers for the distributions. When variability and uncertainty in a quantity are both considered, frequency distributions are used to characterize the variability of the quantity, while there remains uncertainty regarding the frequency distribution. Two-dimensional sampling technique for uncertain frequency distributions is required to generate random numbers. In this study, the two dimensional sampling technique proposed by Frey and Rhodes (1996) is used.

The two dimensional sampling technique developed by Frey and Rhodes (1996) features the use of bootstrap simulation proposed by Efron (1979). The bootstrap technique can quantify the sampling error that is introduced by estimating some statistic of interest from a limited number of sample data points. For example, we have some random points of size n, $\mathbf{x} = \{x_1, x_2, \cdots, x_n\}$, which are from an unknown probability distribution F. The parameter of interest θ, is a characteristic of the distribution F, $\theta = f(F)$, such as mean, standard deviation, or any percentile of the distribution F. An estimate of θ is the statistic $\hat{\theta}$, which is determined from the dataset, $\hat{\theta} = f(x)$. The bootstrap technique can quantify the confidence interval for $\hat{\theta}$. It involves following procedures, according to Frey and Rhodes (1998):

1. Using the data set **x**, the distribution $\hat{F}$ is defined to be an estimate of the unknown population distribution F. The distribution $\hat{F}$ can either be an empirical distribution or a parametric distribution. The former is referred to as nonparametric bootstrap, and the latter as parametric bootstrap;
2. Then, the bootstrap method repeatedly asks the question: what if the data set had been a different set of n random values from the same distribution $\hat{F}$? This question is answered by repeatedly generating bootstrap samples. A bootstrap sample, x^* is defined as a simulated random sample of size n taken from distribution $\hat{F}$. A large number, B, of independent bootstrap samples ($x^*_1, x^*_2, \cdots, x^*_B$) are sampled from the distribution $\hat{F}$. From each of the B bootstrap samples, a new statistic, $\hat{\theta}^*$ is computed. Each $\hat{\theta}^*$ is referred to as a bootstrap replication of $\hat{\theta}$;
3. From the B replication of $\hat{\theta}$s, a confidence interval for $\hat{\theta}$ can be estimated.

Frey and Rhodes (1998) developed a two-dimensional simulation for uncertain frequency distributions by using bootstrap simulation. The overall approach is illustrated in a flow diagram in Figure 2-1. In this approach, bootstrap simulation is first used to generate a total of B paired parameter estimates for the distribution $\hat{F}$. Each pair of parameters represents an alternative frequency distribution for $\hat{F}$. For each alternative frequency distribution, a total of p random samples are simulated to represent one possible realization



Notes:

- B = number of bootstrap replications
- q = sample size used for uncertainty
- p = sample size used for variability

Figure 2-1. Flow Diagram for Bootstrap Simulation and Two-dimensional Simulation of Uncertainty and Variability (Frey and Rhodes, 1998) of variability within the population. Thus, a total of $B \times p$ random numbers are generated, representing p samples from each of B alternative frequency distributions. For each realization of uncertainty (each alternative frequency distribution), the samples are sorted to represent cumulative distribution functions. Thus there are B values for any given statistic (e.g., mean, variance, 95th percentile), which can be used to construct sampling distributions for each statistic.

2.3 Stochastic Optimization and Stochastic Programming

Optimization under uncertainty is generally divided into two categories: stochastic optimization and stochastic programming (Diwekar, *et al.*, 1997). Stochastic optimization problems involve expected value minimization or chance constrained optimization. These problems require that some probabilistic representation of objective functions and constraints be optimized. Stochastic programming deals with the effect of uncertainty on optimal design.

2.3.1 Stochastic Optimization

A general formulation of the stochastic optimization problem can be described as (Diwekar, *et al*., 1997):

Objective: Min or Max $Z=P1\ (f(x, u))$

Subject to: $P2\ (g(x, u)) = 0$

$P3\ (h(x, u)) \leq 0$

Where x are design variables; u are uncertain variables; $P1$, $P2$ and $P3$ are probabilistic functions, which can be expected value, standard deviation, percentile and other statistics; $f\ (x, u)$, $g(x, u)$ and $h(x, u)$ are all functions of x and u.

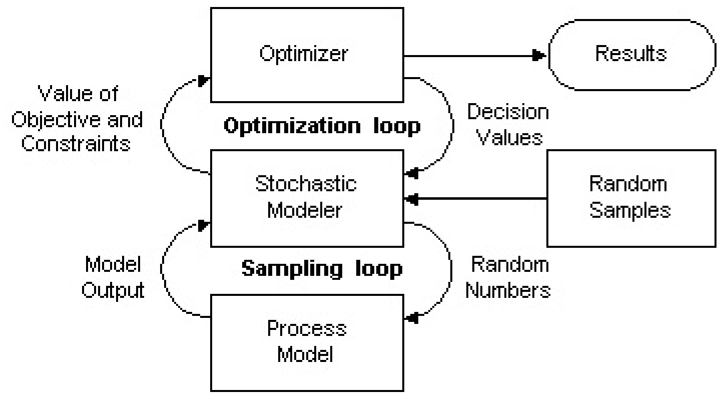


Figure 2-2. Schematic of Stochastic Optimization (adapted from Diwekar, *et al*., 1997)

Stochastic Optimization has been applied to many problems. Watanabe and Ellis (1993) used a stochastic linear model to address an air quality management problem. Shih and Frey (1995) built a stochastic non-linear model for a coal blending problem. However, in the two works, the stochastic optimization problem was analytically transformed to an equivalent deterministic one using chance constrained programming. Therefore the approach they used only applies to certain problems. A general way is to approximate the probabilistic functions through a sampling method (Diwekar, *et al*., 1997). The general way involves two iterative loops: (1) the inner sampling loop and (2) the outer optimization loop. This method has been demonstrated by many researchers (Dantus and High, 1999; Hou *et al*., 2000; Kim and Diwekar, 2000a, 2000b). Figure 2-2 illustrates the coupling of sampling loop and optimization loop in solving a stochastic optimization problem (Diwekar *et al*., 1997).

Figure 2-3 shows the overall flow diagram for doing stochastic optimization. For each pair of design values generated from the optimizer, the process model is run *m* times, where *m* is the number of random values sampled for each uncertain variable). Based on a total of *m* values for each model output, statistics of model output, such as expected value,

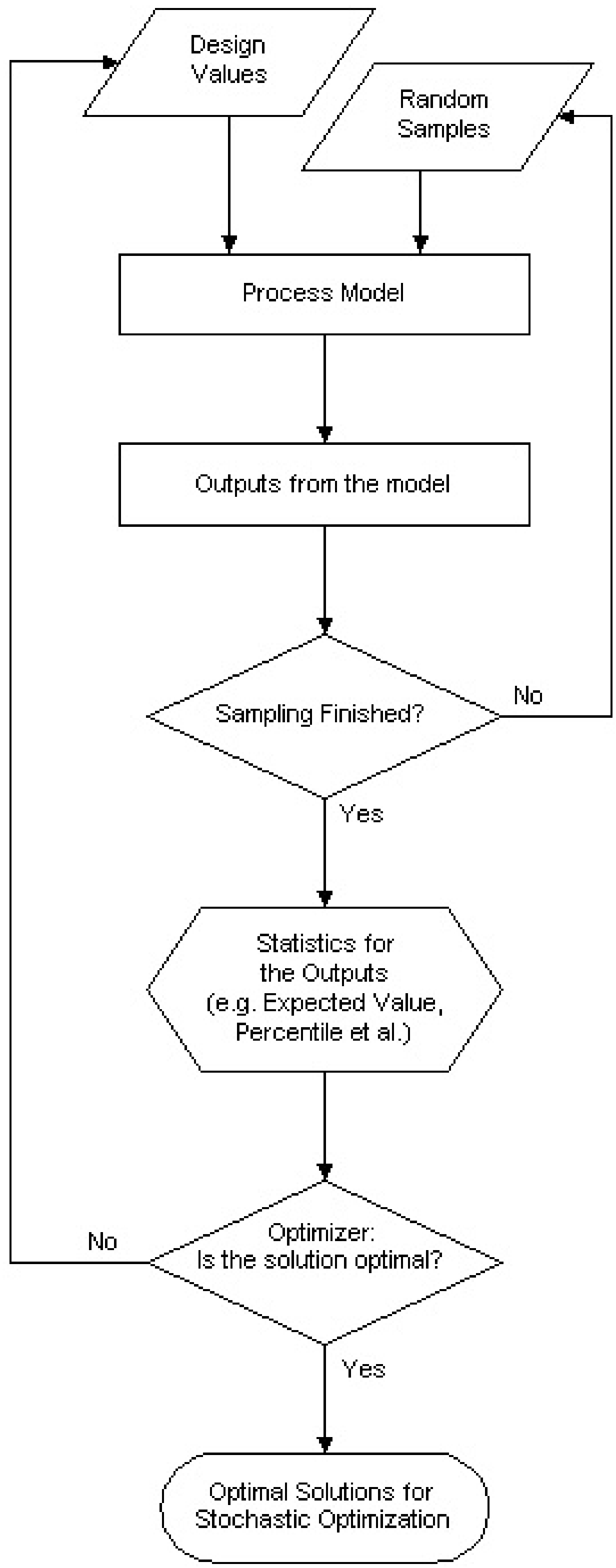


Figure 2-3. Flow Diagram of Stochastic Optimization

variance, or *95*th percentile, can be estimated. These statistics, used as objective function values or constraints, are passed to the optimizer, which either generates new design values or stops to report optimal solutions.

2.3.2 Stochastic Programming

Stochastic programming deals with the effect of uncertainty in model parameters on optimal solutions. Stochastic programming involves deterministic optimization for each random sample of uncertain variables. The formulation of stochastic programming can be represented as (Diwekar, *et al*., 1997):

Objective: Min or Max $Z = z(x, u^*)$

Constraint: $h(x, u^*) = 0$

$g(x, u^*) \leq 0$

Where, x = design variables,

u^* = random sample for uncertain variables,

$z(x, u^*)$, $h(x, u^*)$ and $g(x, u^*)$ = functions of x and u^*.

Stochastic programming involves: (1) an inner optimization loop; and (2) an outer sampling loop. Figure 2-4 shows the coupling of sampling loop and optimization loop involved in stochastic programming (Diwekar *et al*., 1997). The outer sampling loop generates random numbers; for each realization of uncertain variables, the inner optimization loop is run to find the optimal solution. The outputs from stochastic programming form

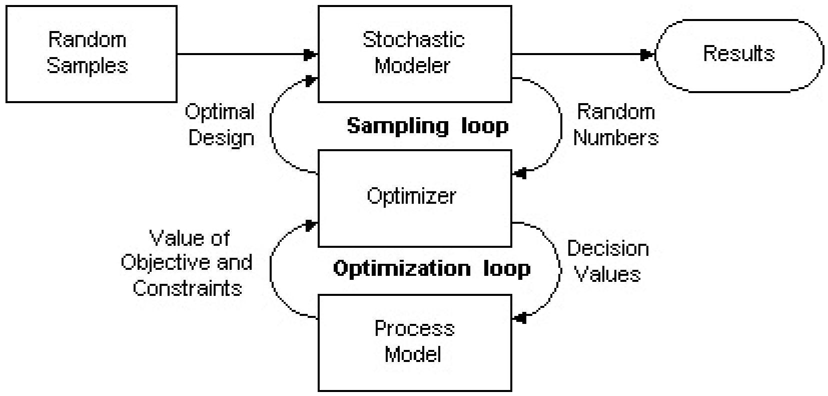


Figure 2-4. Schematic of Stochastic Programming (adapted from Diwekar *et al*., 1997)

probabilistic distributions of optimal solutions. A more detailed flow diagram showing procedures with regard to stochastic programming is given in Figure 2-5. Stochastic programming has been applied to an IGCC system by Diwekar *et al*. (1997). However, because of computational burden associated with the method, this method is rarely used. Some researchers evaluated the effect of uncertainty on optimization solutions. However their work is limited to one uncertain variable at a time (Fournier *et al*., 1999; Pinto, 1998), or to a very small number of simulations (Bak and Tybirk, 1998; Cocks *et al*., 1998).

2.4 Optimization Considering both Variability and Uncertainty

Stochastic optimization and stochastic programming are available for optimization when uncertainty in model parameters is considered. This study extends the stochastic optimization and stochastic programming methods to the situation where both variability and uncertainty in model parameters are considered. Two methods are proposed. The two methods, termed as "coupled stochastic optimization and programming" and "two dimensional stochastic programming" respectively, are based on stochastic optimization and stochastic programming techniques discussed in the previous section.

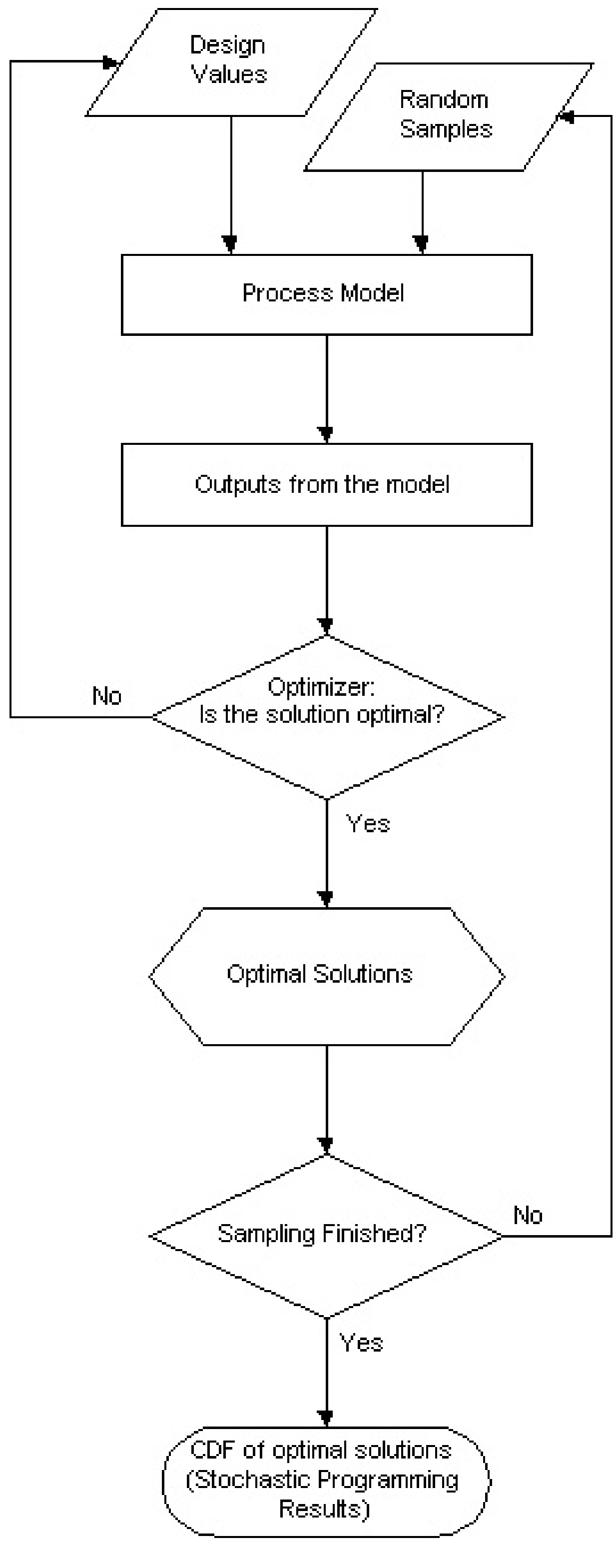


Figure 2-5. Flow Diagram for Stochastic Programming

The coupled stochastic optimization and programming technique involves stochastic optimization for each alternative frequency distribution which represents variability. During each stochastic optimization, a point estimate result for each alternative frequency distribution of model results is optimized. The output of this method is a probability distribution of optimal solutions from stochastic optimization. This method can be used to assess the effect of uncertainty on stochastic optimization results.

Two-dimensional stochastic programming involves deterministic optimization for each sample of variability and uncertainty. The output of this method will be a two dimensional distribution for deterministic optimal solutions. This method enables one to evaluate the effect of both variability and uncertainty on optimal solutions.

The two methods are illustrated by an example in which one variable P among model parameters is assumed to be variable and uncertain and another variable Q among model parameters is assumed to be uncertain.

Let A_{ij} ($1 \leq i \leq m$ and $1 \leq j \leq n$) represents random numbers generated from the two-dimensional sampling technique for the variable P, where m is the realization number for variability and n is the realization number for uncertainty. Let B_j ($1 \leq j \leq n$) represents the random numbers generated from Monte Carlo simulation for the variable Q, where n is the realization number for uncertainty.

The algorithm for coupled stochastic optimization and programming method is described as follows:

1. j=0;

2. $j = j+1$, conduct stochastic optimization for A_{ij} (i from 1 to m) and B_j. A_{ij} (i from 1 to m) means m samples of the j^{th} alternative frequency distribution of P, and B_j

is the j^{th} random sample of Q;

3. If $j < n$, then go back to step 2;

If $j = n$, then stop.

The results are n optimal solutions from stochastic optimization, which can be used to construct a cumulative probability distribution. Figure 2-6 shows a simple schematic of the method. For each realization of uncertainty in variables with both variability and uncertainty, stochastic optimization is done. A detailed flow diagram is given in Figure 2-7.

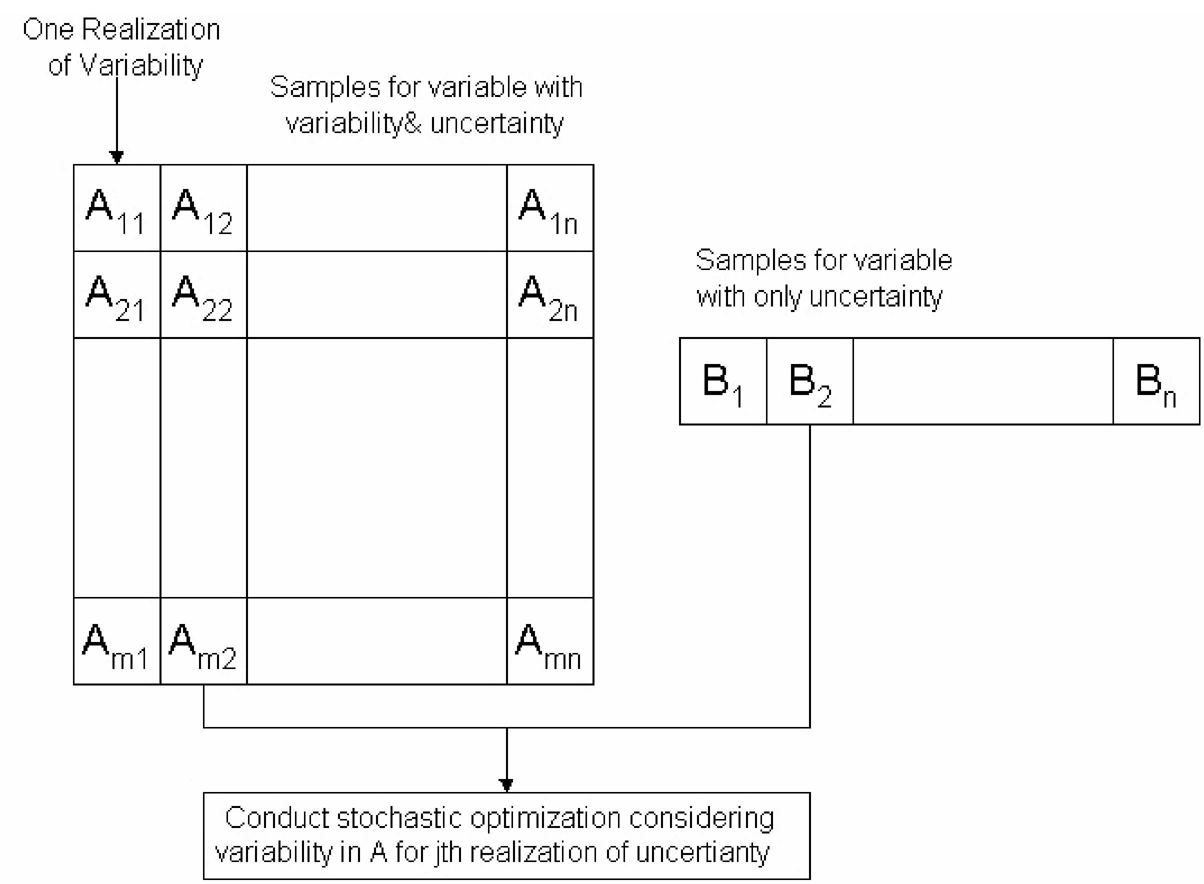


Figure 2-6. Simple Schematic for Coupled Stochastic Optimization and Programming Method

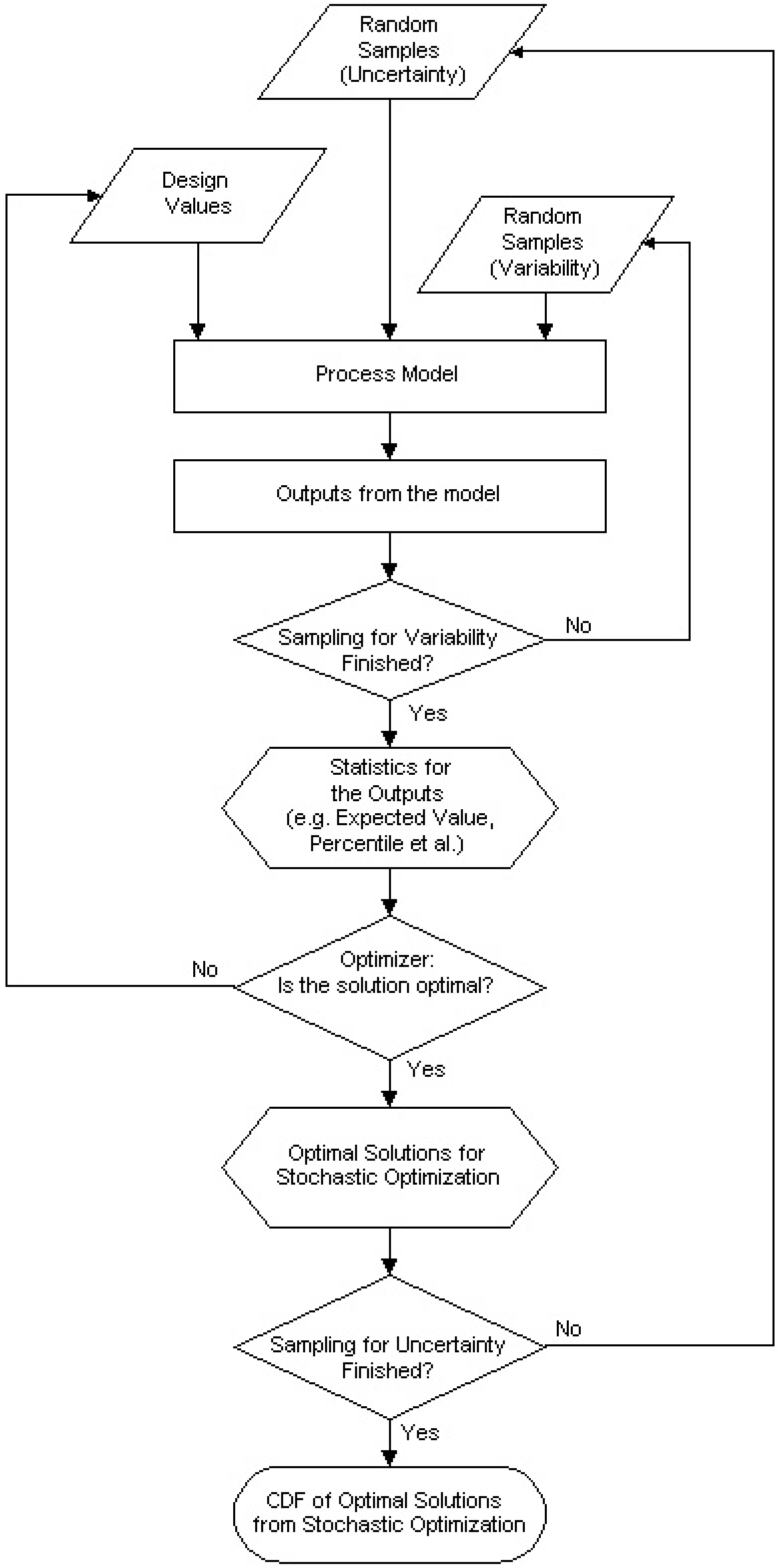


Figure 2-7. Flow Diagram for Coupled Stochastic Optimization and Programming

The algorithm for the two-dimensional stochastic programming technique is described below:

1. j=0;

2. $j = j$ +1 and i=0;

3. $i = i$ +1; for A_{ij} and B_j, conduct deterministic optimization and find the optimal solution;

4. if i<m then go back to step 3, otherwise go forward to step 5;

5. if j<n then go back to step 2, otherwise stop.

The results are $m \times n$ deterministic optimization solutions. Step 3 and step 4 constitute a stochastic programming procedure. Figure 2-8 shows the simple schematic of the method. Detailed flow diagram is given in Figure 2-9.

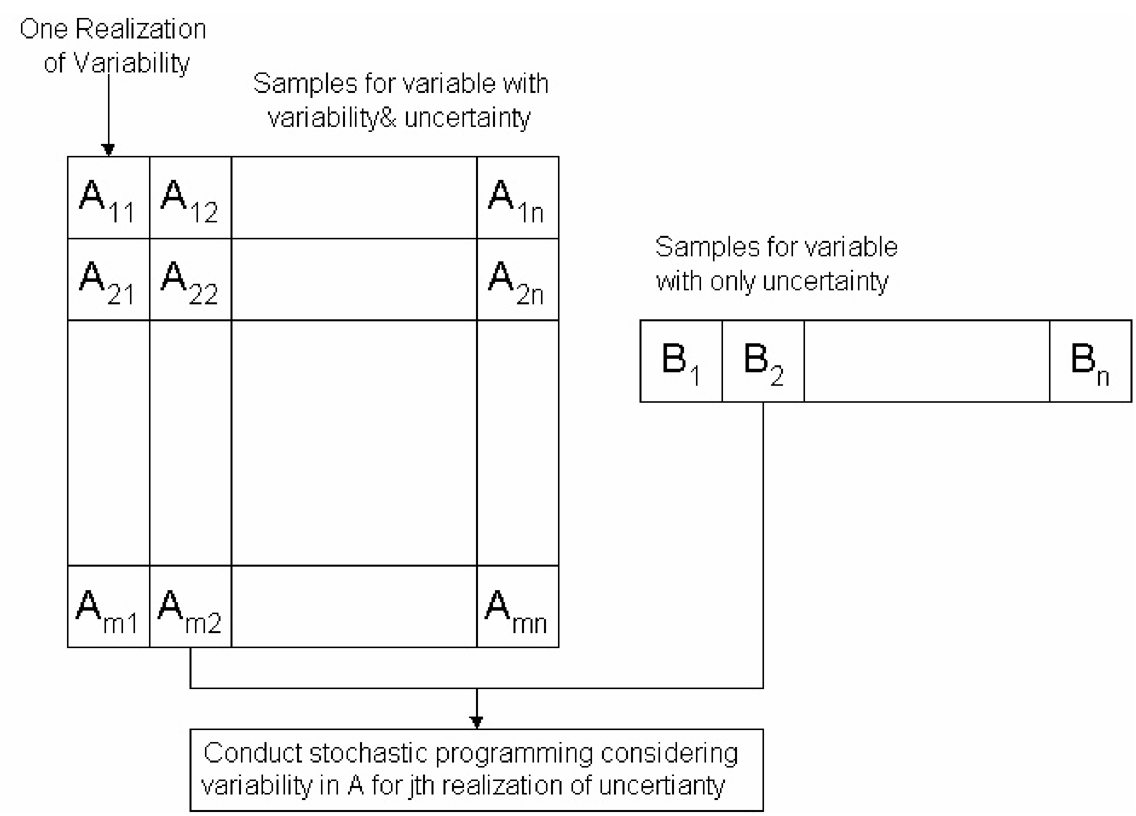


Figure 2-8. Simple Schematic for the Two-dimensional Stochastic Programming Method

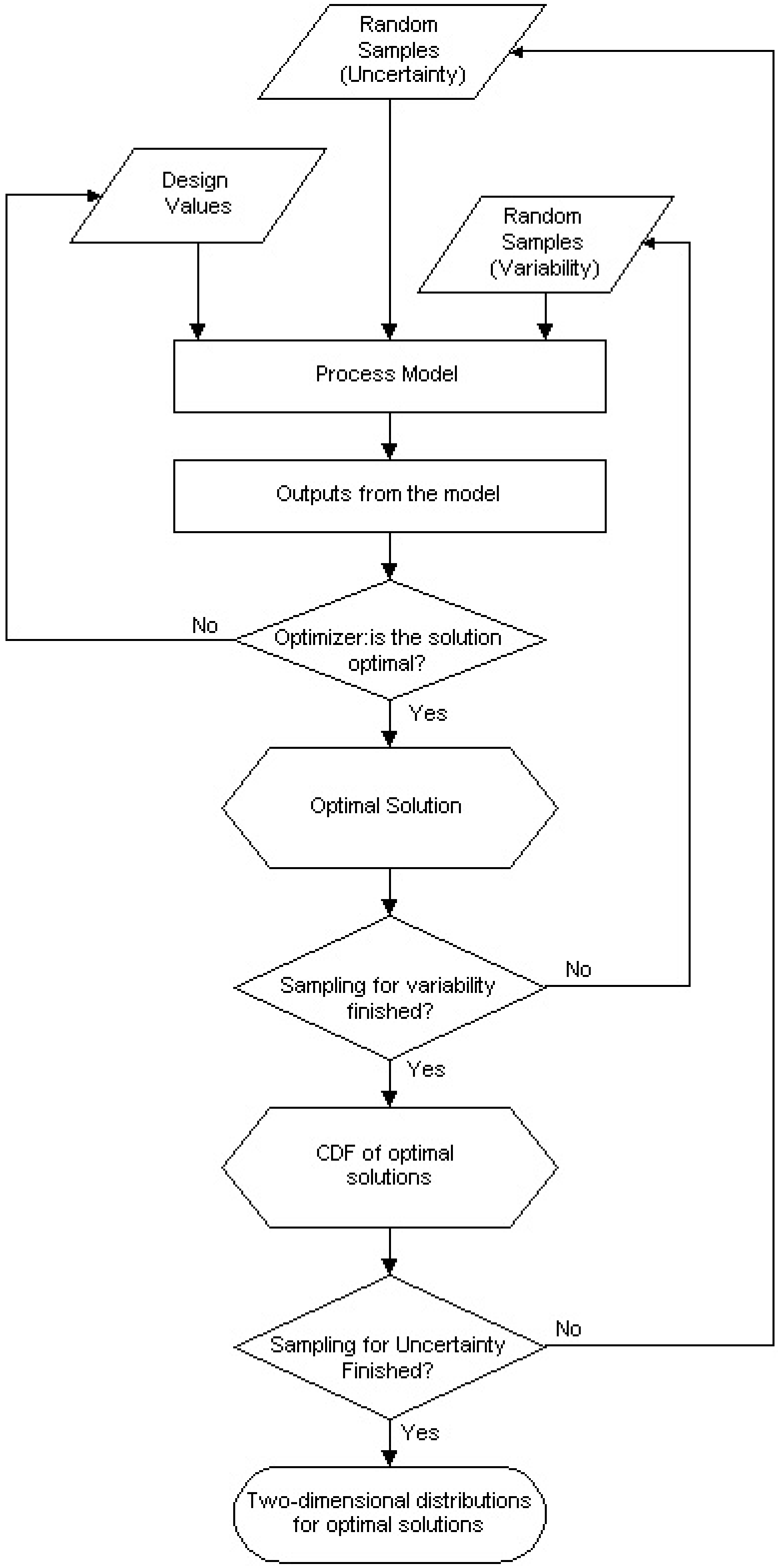


Figure 2-9. Flow Diagram for the Two-dimensional Stochastic Programming Method

3.0 OVERVIEW OF INTEGRATED GASIFICATION COMBINED CYCLE (IGCC) SYSTEM

Environmental regulations are one of the factors that spur the development of new coal-based electric power generation technologies. Conventional emission control systems for a new pulverized coal-fired power plant typically consist of a wet limestone flue gas desulfurization (FGD) system for SO_2 control, an electrostatic precipitator (ESP) for PM removal, and combustion control for NO_X reduction. Selective Catalytic Reduction (SCR) is a post-combustion NO_X control technology that has been demonstrated in Japan, German and a small number of U.S. coal-fired power plants and is expected to be required to comply with the New Source Performance Standard (NSPS) (EPA, 1997). With the stringency of the current NSPS, few new coal plants are currently being built in the U.S.

Integrated Gasification Combined Cycle (IGCC) system is an alternative to the conventional pulverized coal (PC) combustion system. In a combined cycle plant, fuel is burned in a gas turbine, and the hot exhaust gas is used to generate steam for a steam cycle. Electric generators on both the gas turbine and steam turbine generate electricity. IGCC systems are capable of NO_X emissions comparable to or less than those of PC plants equipped with SCR, as well as high levels of SO_2 control (EPRI, 1988). Meanwhile, IGCC systems offer other advantages such as phased construction, fuel flexibility, reduced solid waste, a modular design and a capability to produce useful co-products. The U.S Department of Energy is pursuing development of a new generation of gasification systems intended to offer an environmentally and economically viable alternative for power generation in the U.S. (U.S. DOE, 2000).

Figure 3-1 shows a schematic of an IGCC system (Bharvirkar and Frey, 1998). Coal, steam, and oxygen enter a high pressure, high temperature gasifier reactor vessel. A portion

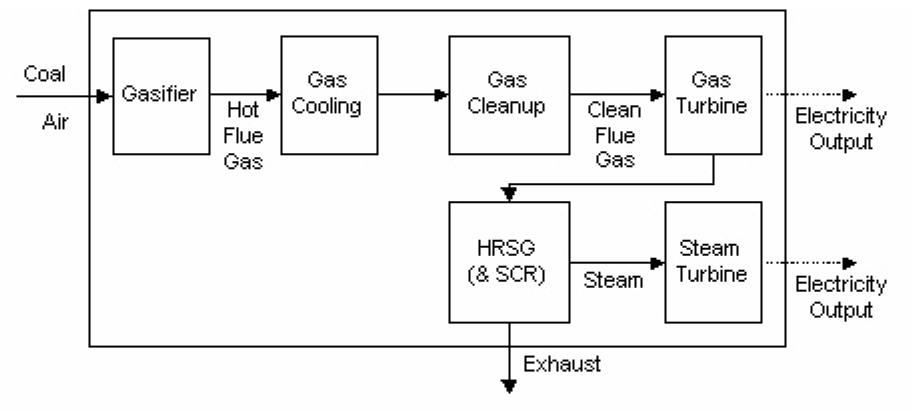


Figure 3-1. Schematic of a KRW-Gasifier based IGCC System with Hot Gas Cleanup

of the coal is combusted to release heat, while the remainder participates in endothermic gasification reactions with steam to produce a syngas containing CO and H_2. The syngas that exits from the gasifier enters a high temperature gas cooling unit, where it is quenched by water. Subsequently it is cleaned of impurities such as particulate matter and sulfur compounds, in the gas cleanup unit.

The clean fuel gas is sent to a gas turbine, where recovered energy is used to rotate generator for electricity. The hot exhaust gas from the gas turbine passes through a Heat Recovery Steam Generator (HRSG). In the HRSG, the syngas is cooled and the transferred heat is used to generate hot boiler feed water, saturated steam, and superheated steam. Superheated steam is used to produce electric power via a steam turbine. Post combustion air pollution control technologies, such as Selective Catalytic Reduction (SCR) for NO_X control, can be located within the HRSG (Frey *et al.*, 1994).

There exist a number of variations of IGCC systems, based primarily on differences in coal gasifier technology. The primary difference in gasifier design is the type of bed in which the coal is gasified. Three general types of gasifiers are moving-bed, fluidized-bed, and entrained-flow (Frey and Rubin, 1990). The IGCC system used as the basis for the case study in this work is a Kellogg-Rust-Westinghouse (KRW) gasifier, which is an example of a fluidized bed (Frey and Rubin, 1990). The KRW-based IGCC systems include a hot gas cleanup system featuring in-bed desulfurization in the gasifier with limestone or dolomite, subsequent sulfur removal from the fuel gas with a zinc ferrite sorbent, a high efficiency cyclone and ceramic filters for particulate removal, sulfation of spent limestone and conversion of carbon remaining in the ash by using a circulating bed boiler (Frey and Rubin, 1992; Frey et al., 1994; Bharvirkar and Frey, 1998).

3.1 Performance, Emissions and Cost Model for KRW Gasifier-based IGCC System

A simplified performance, emissions and cost model of a KRW gasifier-based IGCC system developed by Bharvirkar and Frey (1998) is used in this study. The performance and emissions part of this model is a regression model based on probabilistic analysis of a detailed ASPEN-based model. The accuracy of the simplified model is typically within a percent compared with the ASPEN model (Bharvirkar and Frey, 1998). It provides a selection of four process configurations featuring two gas turbine designs and the inclusion or exclusion of SCR for NO_X control. A description of the four configurations is given in Table 3-1.

In the model, there are 10 independent variables that can be specified by the user, which are shown in Table 3-2. Based on these 10 independent variables, the performance model calculates values for about 60 dependent variables, which are served later as input values to the cost model.

In the original model, the calcium to sulfur ratio (RCAS) for limestone additives to the gasifier is an independent variable. However, in this study, RCAS is no longer treated as an independent variable. According to Diwekar *et al*. (1992), RCAS in the gasifier can be expressed as a function of the sulfur retained in gasifier bottom ash (XSLCNV). In this

Table 3-1. Description of Configurations Considered in the Model

Case	Gas Turbine Pressure Ratio	Gas Turbine Inlet Temperature (°K)	Selective Catalytic Reduction
1	15.0	2350	No
2	15.0	2350	Yes
3	13.5	2300	Yes
4	13.5	2300	No

Table 3-2. Input Variables for the Simplified Performance Model of IGCC System

Variables	Description	Unit	Default Value	Range
CARCNV	Gasifier Carbon Conversion	Fraction	0.95	0.90-0.98
XCRCNV	Carbon Converted in Sulfation Unit	Fraction	0.95	0.90-0.98
RMOXG2C	Gasifier Oxygen to Carbon Ratio	Mole of O2 per Mole of C	0.46	0.45-0.47
RSTM2OX	Gasifier Steam to Carbon Ratio	Mole of H2O Per mole C	0.45	0.445-0.455
RCAS	Calcium to Sulfur Ratio	Mole Ca per mole S	2.60	2.10~3.00
XXCRN	Fraction of Coal bound Nitrogen converted to NH3	Fraction	0.10	0.05 ~ 0.15
XXNH3	Fraction of NH3 converted to NOX in Gas Turbine	Fraction	0.90	0.50~0.90
XSLCNV	Sulfur retained in Gasifier Bottom Ash	Fraction	0.90	0.80-0.95
SCRAE	SCR NOX removal Efficiency	Fraction	0.80	0.50-0.90
XNH3S	SCR NH3 Slip	ppm	10.00	5.00-20.00

(Source: Bharvirkar and Frey, 1998)

work, we adopted this relationship, which is shown in equation 3-1.

$$RCAS = a\left\{\frac{\exp(XSLCNV - b) - 1}{1 - XSLCNV}\right\} \qquad (3\text{-}1)$$

Where, RCAS = calcium to sulfur ratio (mole calcium per mole of sulfur);

XSLCNV = sulfur retained in gasifier bottom ash (fraction);

a=0.233;

b=0.15.

The cost model was developed and updated by Frey and Rubin (Frey and Rubin, 1990; Frey *et al.*, 1994, Frey, 1994). The cost model calculates capital cost, annual fixed operating cost and variable operating cost for 11 process areas, which are coal handling, boiler feed water systems, limestone handling, gas turbine, oxidant feed, heat recovery steam generation, gasification, selective catalytic reduction, zinc ferrite process, steam turbine, sulfation and general facilities.

By default, the original cost model reports cost on the basis of January, 1989. In this work, the model is modified to report the cost on the basis of January, 2002, by using chemical engineering plant cost index (CI) and industrial chemicals producer price index (CICPPI) for January, 2002, which are 390.3 and 417.95, respectively (Chemical Week Publish, 2002). These values are not substantially different from those of January, 1989. CI for January of 2002 is only 10% higher than that of January, 1989 which is 354.7. CICPPI for January of 2002 is 6.6% higher than that of January, 1989 which is 391.87.

3.2 Interface of the Model

The original performance, emissions and cost model accepts input values through an interactive interface. To enable the data exchange between the model and other programs during simulation and optimization, the model is changed to accept input values through an input file, and to report output values through an output file. The input file includes values for all variables that might be used as design variables, or treated as variables with variability and/or uncertainty. A summary of input variables is given in Table 1 of Appendix A. An example of an input file is also given. The output file includes values that are of interest in optimization problem. A summary of output variables is given in Table A-2 of Appendix A. An example of output file is also given.

3.3 Variability and Uncertainty in Model Inputs

For the IGCC model discussed above, 27 variables were identified as uncertain variables. For each uncertain variable, probabilistic distribution is used to characterize its uncertainty. The selection of these variables and development of uncertainty assumptions are mainly based on the work by Frey et al. (1994). They identified and estimated uncertainties for these parameters based on literature review, data analysis, and elicitation of expert judgments from engineers involved in IGCC technology development at DOE's Morgantown Energy Technology Center (DOE/METC) (Frey et al., 1994). Table 3-3 summarizes the distribution assumptions for the uncertain variables.

Another 26 performance and cost inputs of the model were identified to have both variability and uncertainty. The selection of these variables is based on the work by Frey and Rubin (1991), and Frey *et al.* (1994). They identified these parameters based on literature review, data analysis, and elicitation of expert judgments from engineers involved in IGCC technology development at DOE's Morgantown Energy Technology Center (DOE/METC) (Frey and Rubin, 1991; Frey et al., 1994). Similarly, for these variables with both variability and uncertainty, probabilistic distributions are assigned to represent the variability. Table 3-4 shows the assumed distributions for these variables and the references for these assumptions.

Table 3-3. Distribution Assumptions for Uncertain Variables in the IGCC Model

Description of the variables	Default value	Distribution assumptions [a]	Reference
Factor of Engineering and home office fee	0.10	T: 0.07-0.13 (0.10)	Frey *et al*. (1994)
Indirect Construction cost factor	0.20	T: 0.15-0.25 (0.20)	Frey *et al*. (1994)
Project contingency factor	0.175	U: 0.10-0.25	Frey *et al*. (1994)
Unit cost of coal ($/$10^6$Btu)	1.61	N (1, 0.05) [b]	Expert Judgment
Unit cost of Sulfuric acid ($/ton)	110	N (1, 0.05) [b]	Expert Judgment
Unit cost of NaOH ($/ton)	220	N (1, 0.05) [b]	Expert Judgment
Unit cost of Na2HPO4 ($/lb)	0.7	N (1, 0.05) [b]	Expert Judgment
Unit cost of Hydrazine ($/lb)	3.2	N (1, 0.05) [b]	Expert Judgment
Unit cost of Morpholine ($/lb)	1.3	N (1, 0.05) [b]	Expert Judgment
Unit cost of Lime ($/ton)	80	N (1, 0.05) [b]	Expert Judgment
Unit cost of Soda Ash ($/ton)	160	N (1, 0.05) [b]	Expert Judgment
Unit cost of Corrosion Inh. ($/lb)	1.9	N (1, 0.05) [b]	Expert Judgment
Unit cost of Surfactant ($/lb)	1.25	N (1, 0.05) [b]	Expert Judgment
Unit cost of Chlorine ($/ton)	250	N (1, 0.05) [b]	Expert Judgment
Unit cost of Biocide ($/lb)	3.6	N (1, 0.05) [b]	Expert Judgment
Unit cost of Plant Air Ads ($/lb)	2.8	N (1, 0.05) [b]	Expert Judgment
Unit cost of LPG Flare ($/bbl)	11.7	N (1, 0.05) [b]	Expert Judgment
Unit cost of Waste Water ($/gpm ww)	840	N (1, 0.05) [b]	Expert Judgment
Unit cost of Fuel Oil ($/bbl)	42	N (1, 0.05) [b]	Expert Judgment
Unit cost of Raw Water ($/K gal)	0.73	N (1, 0.05) [b]	Expert Judgment
Unit cost of Limestone ($/ton)	18	T: 18-25 (18)	Frey *et al*. (1994)
Zinc Ferrite sorbent sulfur loading, wt-% sulfur in sorbent	17	N (17, 4.82)	Frey *et al*. (1994)
Zinc Ferrite sorbent attrition rate, wt-% sorbent loss per cycle	1	F: 0.17-0.34 (5%); 0.34-0.5 (20%); 0.5-1 (25%); 1-1.5 (25%); 1.5-5 (20%); 5-25 (5%)	Frey *et al*. (1994)
Error Term of HRSG direct cost model, $Million	0	N(0, 5.62)	Frey *et al*. (1994)
Error Term of SCR direct cost model, $Million	0	N(0, 0.0422)	Frey *et al*. (1994)
Error Term of Steam Turbine, $ Million	0	N(0, 5.13)	Frey *et al*. (1994)

[a]: T=Triangular distribution, lower bound and upper bound are given, mode is in parenthesis;
U=Uniform distribution, lower and upper bound are given;
N=Normal distribution, mean value and standard deviation are given;
F=Fractile distribution, lower and upper bound of each range are given, along with the possibility of samples within that range;

[b]: on a relative basis, which means random samples from the distribution should be multiplied with default value

Table 3-4: Distribution Assumptions for the Variables with both Variability and Uncertainty in the IGCC Model

Variable Name	Description	Default Value	Distribution Assumptions for variability [a]	Reference
CARCNV	Gasifier Carbon Conversion	0.95	T: 0.90-0.98 (0.95)	Frey *et al*. (1994)
XCRCNV	Carbon Converted in sulfation unit	0.95	T:0.90-0.98 (0.95)	Frey *et al*. (1994)
XXCRN	Fraction of coal bound nitrogen converted to NH3	0.1	T: 0.05-0.15 (0.1)	Frey *et al*. (1994)
XXNH3	Fraction of NH_3 converted to NO_X in Gas Turbine	0.9	T: 0.5-0.9 (0.9)	Frey *et al*. (1994)
ALABOR	Average labor rate, including burdens ($/hour)	19.7	N(19.7,0.647)	Frey *et al*. (1994)
Contingencies of Process Areas				
FPCCH	Coal handling	0.05	U: 0.00-0.10	Frey and Rubin (1991)
FPCL	Limestone handling	0.05	U:0.00-0.10	Frey and Rubin (1991)
FPCOF	Oxidant feed	0.10	U: 0.00-0.20	Frey and Rubin (1991)
FPCG	Gasification	0.2	T: 0.0-0.4 (0.2)	Frey and Rubin (1991)
FPCS	Sulfation	0.4	T: 0.20-0.60 (0.4)	Frey and Rubin (1991)
FPCZF	Zinc ferrite	0.4	U: 0.00-0.80	Frey and Rubin (1991)
FPCGT	Gas turbine	0.25	U: 0.00-0.50	Frey and Rubin (1991)
FPCHR	Heat recovery steam generator	0.025	U: 0.000-0.050	Frey and Rubin (1991)
FPCCR	Selective catalytic reduction	0.1	U: 0.00-0.2	Frey and Rubin (1991)
FPCST	Steam turbine	0.025	U: 0.00-0.05	Frey and Rubin (1991)
FPCGF	General facilities	0.05	U: 0.00-0.10	Frey and Rubin (1991)
Maintenance Factors of Process Areas				
FMCOF	Oxidant feed	0.02	T: 0.01-0.03 (0.02)	Frey and Rubin (1991)
FMCG	Gasification	0.045	T:0.03-0.06 (0.045)	Frey and Rubin (1991)
FMCS	Sulfation	0.04	T: 0.03-0.06 (0.04)	Frey and Rubin (1991)
FMCZF	Zinc ferrite	0.03	T: 0.03-0.06 (0.03)	Frey and Rubin (1991)
FMCGT	Gas turbine	0.02	T:0.015-0.06 (0.02)	Frey and Rubin (1991)
FMCCR	Selective catalytic reduction	0.02	T: 0.01-0.03 (0.02)	Frey *et al*. (1994)
Unit Cost of Materials				
BCCSRC	SCR catalyst ($/ft^3)	250	T:250-660 (350)	Frey *et al*. (1994)
BCNH3	Ammonia ($/ton)	150	U(150, 225)	Frey *et al*. (1994)
BCZFSO	Zinc Ferrite sorbent ($/lb)	3.00	T: 0.75-5.00 (3.00)	Frey *et al*. (1994)
BCASHD	Unit cost of Ash Disposal ($/ton)	10	T: 10-25 (10)	Frey *et al*. (1994)

[a]: T=Triangular distribution, lower bound and upper bound are given, mode is in parenthesis;
U=Uniform distribution, lower and upper bound are given;
N=Normal distribution, mean value and standard deviation are given;

Initially, bootstrap simulation was used to generate samples for variables with both variability and uncertainty according to the assumptions in Table 3-4. It was found that bootstrap samples in many cases exceed the range of the variables. For example, gasifier carbon conversion (CARCNV) is assigned a triangular distribution for variability and is bounded by 0.90 and 0.98. However, bootstrap samples in some cases are lower than 0.90 or higher than 0.98, which causes the IGCC model not to work correctly. To resolve this problem, distributions in Table 3-4 are transformed to beta distribution. For example, variable X is constrained by a lower bound of a and an upper bound of b. X is first transformed to X' by Equation (3-2). Thus, X' is bounded by 0 and 1. Variability in X' is represented by a beta distribution. When bootstrap samples are generated for X', X can be calculated from X' by Equation (3-3). Since bootstrap samples for beta distribution are strictly bounded by 0 and 1, samples for X are strictly bounded within a and b.

$$X' = (X - a)/(b - a) \qquad (3\text{-}2)$$

$$X = a + (b - a) \times X' \qquad (3\text{-}3)$$

For those variables with uniform distributions, the transformed variable X' is a uniform distribution within 0 and 1. Thus, a beta distribution with parameters beta(1,1) can be used for X', since this beta distribution is the same as a uniform distribution between 0 and 1. For other variables which are not uniform distributions, a procedure was developed for determining the corresponding parameters of a beta distribution for X'. For each of these variables, 100 random samples were generated from the original distribution. These random numbers were transformed according to Equation (3-2). A beta distribution was fitted to the transformed samples. The goodness-of-fit was assessed by the Kolmogorov-Smirnov (KS) test, which is a common testing method (Cullen and Frey, 1999). The fitted beta distribution is the assumed distribution for X'. For example, gasifier carbon conversion (CARCNV) has a triangular distribution bounded by 0.90 and 0.98. First, 100 random numbers were generated from this triangular distribution. The random samples were transformed according to Equation (3-2). The transformed samples were fitted to a beta distribution, which was found to be beta(2.5, 2.1). In this case, beta(2.5, 2.1) is used as distribution for X' of CARCNV.

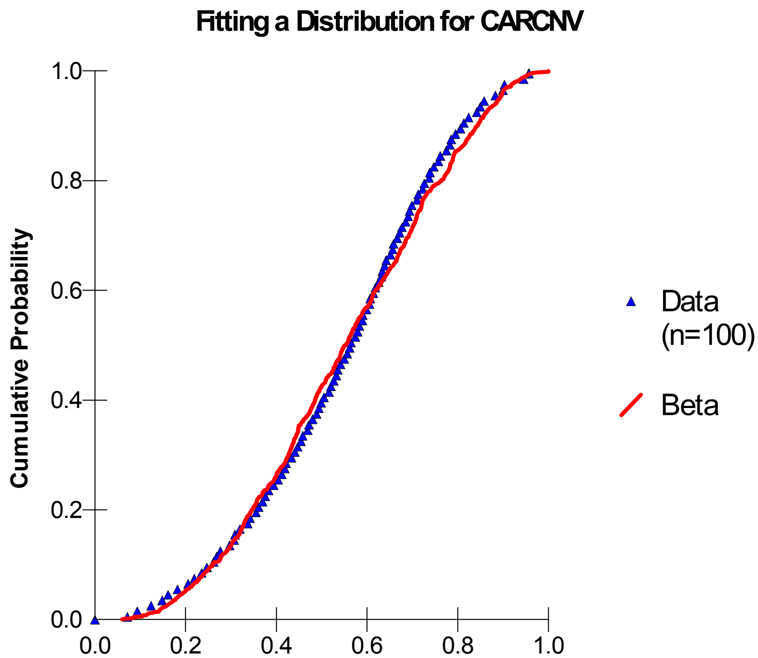


Figure 3-2. Fitting of Beta Distribution to Random Numbers (transformed to be between 0 and 1) from Original Triangular Distribution of CARCNV

Figure 3-2 shows the fitted beta(2.5, 2.1) distribution compared to the transformed random samples. The beta(2.5, 2.1) distribution fits the random samples very well. The KS Test was used to determine whether the fit is good. In this case, the K-S statistics is 0.031, which is lower than the critical value of 0.088, thus indicating a good fit.

Table 3-5 summarizes the transformed distributions for variables with variability. For each variable, beta distributions were found to approximate the original distribution assumptions very well. Table 3-6 summarizes K-S testing results for each variable. Each fitting passes the K-S test, indicating good fit. The transformed distributions, not the original distributions shown in Table 3-4, are used in this study.

Another effort in this work is to quantify the uncertainty in the mean of the variables with both variability and uncertainty. To do this, bootstrap simulation is run for each

Table 3-5. Distribution Assumptions for the Variables with both Variability and Uncertainty in the IGCC Model

Variable Name	Description	Original Distribution for variability [a]	Transformed Distribution for variability [b]
CARCNV	Gasifier Carbon Conversion	T: 0.90-0.98 (0.95)	0.90 + 0.08* Beta (2.6, 2.2)
XCRCNV	Carbon Converted in sulfation unit	T:0.90-0.98 (0.95)	0.90 + 0.08*Beta (2.6, 2.2)
XXCRN	Fraction of coal bound nitrogen converted to NH3	T: 0.05-0.15 (0.1)	0.05 + 0.10*Beta (2.5, 2.5)
XXNH3	Fraction of NH_3 converted to NO_X in Gas Turbine	T: 0.5-0.9 (0.9)	0.5 + 0.4*Beta (2.0, 1.0)
ALABOR	Average labor rate, including burdens ($/hour)	N(19.7,0.647)	Normal (19.7, 0.649)
Contingencies of Process Areas			
FPCCH	coal handling	U: 0.00-0.10	0.10* Beta(1,1)
FPCL	limestone handling	U:0.00-0.10	0.10* Beta(1,1)
FPCOF	oxidant feed	U: 0.00-0.20	0.20* Beta(1,1)
FPCG	gasification	T: 0.0-0.4 (0.2)	0.20* Beta(2.5,2.5)
FPCS	sulfation	T: 0.20-0.60 (0.4)	0.20+ 0.40* Beta(2.5,2.5)
FPCZF	zinc ferrite	U: 0.00-0.80	0.80* Beta(1,1)
FPCGT	gas turbine	U: 0.00-0.50	0.50* Beta(1,1)
FPCHR	heat recovery steam generator	U: 0.000-0.050	0.050* Beta(1,1)
FPCCR	selective catalytic reduction	U: 0.00-0.2	0.20* Beta(1,1)
FPCST	steam turbine	U: 0.00-0.05	0.05* Beta(1,1)
FPCGF	general facilities	U: 0.00-0.10	0.10* Beta(1,1)
Maintenance Factors of Process Areas			
FMCOF	oxidant feed	T: 0.01-0.03 (0.02)	0.01+0.02* Beta(2.5,2.5)
FMCG	gasification	T: 0.03-0.06 (0.045)	0.03+0.03* Beta(2.5,2.5)
FMCS	sulfation	T: 0.03-0.06 (0.04)	0.03+0.03* Beta(2.1, 2.6)
FMCZF	zinc ferrite	T: 0.03-0.06 (0.03)	0.03+0.03* Beta(1.0,2.0)
FMCGT	gas turbine	T: 0.015-0.06 (0.02)	0.015+0.045* Beta(1.3, 2.3)
FMCCR	selective catalytic reduction	T: 0.01-0.03 (0.02)	0.01+0.02* Beta(2.5,2.5)
Unit Cost of Materials			
BCCSRC	SCR catalyst ($/ft^3)	T:250-660 (350)	250+410* Beta(1.6, 2.1)
BCNH3	Ammonia ($/ton)	U(150, 225)	150+75* Beta(1,1)
BCZFSO	Zinc Ferrite Sorbent ($/lb)	T: 0.75-5.00 (3.00)	0.75+4.25* Beta (2.5, 2.3)
BCASHD	Unit cost of Ash Disposal ($/ton)	T: 10-25 (10)	10 +15* Beta (1.0, 2.0)

[a]: T=Triangular distribution, lower bound and upper bound are given, mode is in parenthesis;
U=Uniform distribution, lower and upper bound are given.

[b]: Normal = Normal distribution, mean value and standard deviation are given in parenthesis;
Beta = Beta distribution, shape parameters are given in parenthesis.

Table 3-6. K-S Test Results of Beta Distributions fitted to Transformed Random Samples from Original Distributions of Variability

Variable Name	Original Distribution [a]	Original distribution transformed to within 0 and 1 [a]	Fitted Beta distribution [a]	K-S Test [b]	K-S Test pass/failed? [c]
CARCNV	T: 0.90-0.98 (0.95)	T: 0-1 (0.625)	Beta (2.6, 2.2)	0.031	Passed
XCRCNV	T:0.90-0.98 (0.95)	T: 0-1 (0.625)	Beta (2.6, 2.2)	0.030	Passed
XXCRN	T: 0.05-0.1(0.1)	T: 0-1 (0.5)	Beta (2.5, 2.5)	0.023	Passed
XXNH3	T: 0.5-0.9 (0.9)	T: 0-1 (1)	Beta (2.0, 1.0)	0.013	Passed
FPCCH	U: 0.00-0.10	U: 0-1	Beta(1,1)	0.012	Passed
FPCL	U:0.00-0.10	U: 0-1	Beta(1,1)	0.012	Passed
FPCOF	U: 0.00-0.20	U: 0-1	Beta(1,1)	0.013	Passed
FPCG	T: 0.0-0.4 (0.2)	T: 0-1 (0.5)	Beta(2.5,2.5)	0.025	Passed
FPCS	T: 0.20-0.60 (0.4)	T: 0-1 (0.5)	Beta(2.5,2.5)	0.026	Passed
FPCZF	U: 0.00-0.80	U: 0-1	Beta(1,1)	0.012	Passed
FPCGT	U: 0.00-0.50	U: 0-1	Beta(1,1)	0.012	Passed
FPCHR	U: 0.000-0.050	U: 0-1	Beta(1,1)	0.012	Passed
FPCCR	U: 0.00-0.2	U: 0-1	Beta(1,1)	0.013	Passed
FPCST	U: 0.00-0.05	U: 0-1	Beta(1,1)	0.012	Passed
FPCGF	U: 0.00-0.10	U: 0-1	Beta(1,1)	0.013	Passed
FMCOF	T: 0.01-0.03 (0.02)	T: 0-1 (0.5)	Beta(2.5,2.5)	0.025	Passed
FMCG	T: 0.03-0.06 (0.045)	T: 0-1 (0.5)	Beta(2.5,2.5)	0.025	Passed
FMCS	T: 0.03-0.06 (0.04)	T: 0-1 (0.333)	Beta(2.1, 2.6)	0.032	Passed
FMCZF	T: 0.03-0.06 (0.03)	T: 0-1 (0)	Beta(1.0,2.0)	0.012	Passed
FMCGT	T: 0.015-0.06 (0.02)	T: 0-1 (0.11)	Beta(1.3, 2.3)	0.039	Passed
FMCCR	T: 0.01-0.03 (0.02)	T: 0-1 (0.5)	Beta(2.5,2.5)	0.024	Passed
BCSCRC	T:250-660 (350)	T:0-1 (0.244)	Beta(1.6, 2.1)	0.046	Passed
BCNH3	U(150, 225)	U:0-1	Beta(1,1)	0.012	Passed
BCZFSO	T: 0.75-5.00 (3.00)	T: 0-1 (0.53)	Beta (2.5, 2.3)	0.027	Passed
BCASHD	T: 10-25 (10)	T:0-1 (0)	Beta (1.0, 2.0)	0.012	Passed

[a]: T=Triangular distribution, lower bound and upper bound are given, mode is in parenthesis
U=Uniform distribution, lower and upper bound are given;
Beta = Beta distribution, shape parameters are given in parenthesis.

[b]: Kolmogorov-Smirnov Test of beta distribution to transformed random samples (according to Equation 3-2) from original distributions.

[c]: Critical value of K-S test for each fit is 0.088.

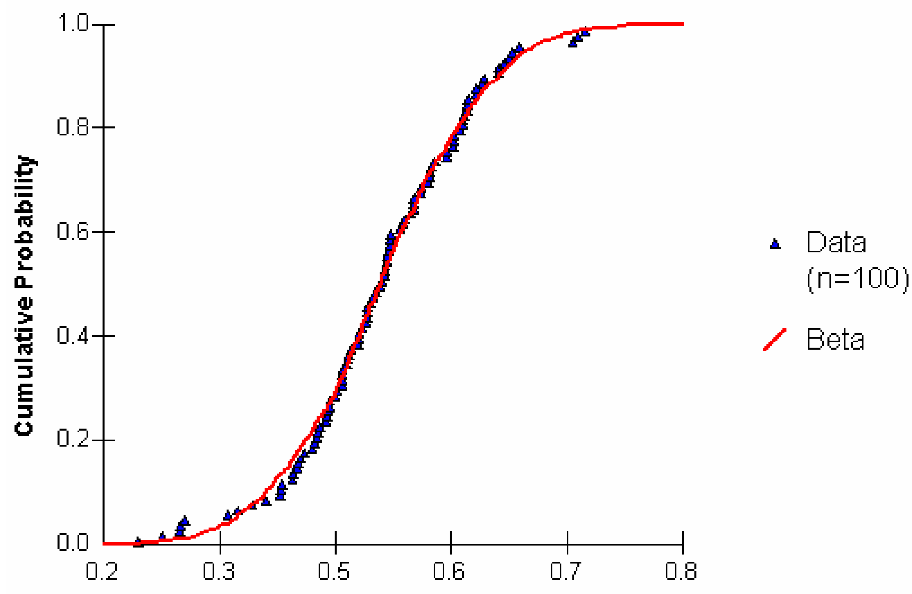


Figure 3-3. Fitting of Beta (14.8, 14.8) Distribution to the 100 Mean Values of Bootstrap Samples from Beta (1.0, 1.0) Distribution

variable according to the beta distributions shown in Table 3-5 (The number of bootstrap replicates is 100, and the sample size for simulation of variability is 100). Although it is desirable to use a larger number of bootstrap replications, it was not practical to do so given the computational requirements. Since there are 100 bootstrap replicates, there are a total of 100 mean values for each such input. These 100 numbers are fitted to a beta distribution, which through transformation by Equation (3-3), is used to represent the uncertainty in the mean of the variables with both variability and uncertainty. For example, Figure 3-3 shows the fitted beta (14.8, 14.8) distribution to the 100 mean values of the bootstrap samples from beta (1.0, 1.0) distribution. The K-S test statistics was 0.049, which is lower than the critical value of 0.088, thus indicating a good fit. Table 3-7 summarizes the uncertainty in the mean of the variables with both variability and uncertainty. Table 3-8 summarizes K-S testing results for each fit.

Table 3-7. Distribution Assumptions for Uncertainties in the Mean Value of the Variables with both Variability and Uncertainty in the IGCC Model

Variable Name	Description	Distribution Assumptions [a]	K-S Test [b]	K-S Test Passed/Failed [c]
CARCNV	Gasifier Carbon Conversion	0.90 + 0.08* Beta (30, 25)	0.044	Passed
XCRCNV	Carbon Converted in sulfation unit	0.90 + 0.08* Beta (27, 22)	0.042	Passed
XXCRN	Fraction of coal bound nitrogen converted to NH3	0.05 + 0.10* Beta (30, 30)	0.039	Passed
XXNH3	Fraction of NH_3 converted to NO_X in Gas Turbine	0.5 + 0.4* Beta (37, 17)	0.047	Passed
ALABOR	Average labor rate, including burdens ($/hour)	Normal (19.7, 0.065)	0.053	Passed
Contingencies of Process Areas				
FPCCH	Coal handling	0.10* Beta (14.8,14.8)	0.049	Passed
FPCL	Limestone handling	0.10* Beta (14.8,14.8)	0.049	Passed
FPCOF	Oxidant feed	0.20* Beta (14.8,14.8)	0.049	Passed
FPCG	Gasification	0.20* Beta (29.5,29.5)	0.039	Passed
FPCS	Sulfation	0.20+ 0.40* Beta (29.5,29.5)	0.039	Passed
FPCZF	Zinc ferrite	0.80* Beta (14.8,14.8)	0.049	Passed
FPCGT	Gas turbine	0.50* Beta (14.8,14.8)	0.049	Passed
FPCHR	Heat recovery steam generator	0.050* Beta (14.8,14.8)	0.049	Passed
FPCCR	Selective catalytic reduction	0.20* Beta (14.8,14.8)	0.049	Passed
FPCST	Steam turbine	0.05* Beta (14.8,14.8)	0.049	Passed
FPCGF	General facilities	0.10* Beta (14.8,14.8)	0.049	Passed
Maintenance Factors of Process Areas				
FMCOF	Oxidant feed	0.01+0.02* Beta (30,30)	0.039	Passed
FMCG	Gasification	0.03+0.03* Beta (30,30)	0.039	Passed
FMCS	Sulfation	0.03+0.03* Beta (23, 30)	0.051	Passed
FMCZF	Zinc ferrite	0.03+0.03* Beta (30,43)	0.058	Passed
FMCGT	Gas turbine	0.015+0.045* Beta (13, 22)	0.047	Passed
FMCCR	Selective catalytic reduction	0.01+0.02* Beta (29.5,29.5)	0.039	Passed
Unit Cost of Materials				
BCCSRC	SCR catalyst ($/ft^3)	250+410* Beta (1.8, 2.5)	0.060	Passed
BCNH3	Ammonia ($/ton)	150+75* Beta (14.8,14.8)	0.039	Passed
BCZFSO	Zinc Ferrite Sorbent ($/lb)	0.75+4.25* Beta (32,32)	0.048	Passed
BCASHD	Unit cost of Ash Disposal ($/ton)	10 +15* Beta (10, 20)	0.037	Passed

[a]: Beta = Beta distribution, shape parameters are given in parenthesis.

[b]: Kolmogorov-Smirnov Test of beta distribution to mean values of bootstrap samples of each variable.

[c]: Critical value of K-S test for each fit is 0.088.

4.0 SOFTWARE IMPLEMENTATION

This chapter discusses the software implementation for doing optimization under variability and/or uncertainty. Optimization of process models under variability and/or uncertainty includes three parts: random number generator, optimization solver, and the process model. The process model used in this study is a simplified performance, emissions and cost model for a KRW gasifier based IGCC system, and has been introduced in Chapter 3. In this Chapter, the random number generator, optimization solver, and how the three parts are integrated into a single framework are discussed.

4.1 Random Number Generator

In this study, random numbers for variability, uncertainty, or both variability and uncertainty in parameters are generated through an existing software ―AuvTool (Analysis of Uncertainty and Variability Tool). AuvTool was developed by Zheng and Frey (2002). It uses a two-dimensional sampling method featuring bootstrap simulation for simultaneously simulating variability and uncertainty. This technique was proposed by Frey and Rhodes (1996), and has been discussed in Chapter 2. AuvTool can also generate one-dimensional samples representing only variability or uncertainty based on Monte Carlo simulation. AuvTool uses combined Multiple Recursive Generators (MRGs) presented by L'Ecuyer (1996) as a pseudo-random number generator (Frey *et al*., 2002). Random numbers generated from AuvTool are saved as a Microsoft Excel file. Through this file, random samples are read and used in the optimization process.

4.2 Overview of the Optimizer

Evolver is chosen as the optimization solver in this study. Evolver is a genetic algorithm (GA) based optimizer developed by Palisade Corporation (Palisade, 1998).

4.2.1 Overview of Genetic Algorithms

Genetic algorithm (GA) is a powerful stochastic search and optimization technique based on principles from evolution theory. Holland (1975) pioneered the development of GA. In recent years, GA has been widely applied to many fields, such as air quality management (Loughlin *et al*., 2000), chemical processes or equipment design (Wang *et al*., 1996; Tayal *et al*. 1999), and water resource management (Wardlaw and Sharif, 1999; Burn and Yulianti, 2001).

In GA, each potential solution to the problem is analogous to an organism or an individual and is encoded as a chromosome. A fitness value is associated with each individual to determine how "good" it is, which is based on the objective function value of the individual and its satisfaction with the constraints. GA considers a number of these individuals simultaneously, which is termed as a population or generation. GA starts with an initial population that is randomly generated. Then GA undergoes probabilistic operations, including crossover, mutation and selection. Crossover is the main genetic operator. It operates on two parent chromosomes (or individuals) and generates offspring by combining both chromosomes' features. A simple way for crossover is to exchange a gene segment between two parents to generate offspring. Mutation is achieved by randomly replacing part of gene in an individual with new randomly generated gene information. Crossover and mutation occur randomly for an individual in the population; however these processes occur according to some possibilities which are defined as crossover and mutation rate respectively. After a specified number of realizations of crossover and mutation for the current population, selection is made based on the fitness of each individual, upon completion of which, a new population or generation with same size as the former one, is formed. With each generation, the average fitness of individuals will be improved. This process of crossover, mutation and selection is repeated until some stopping criteria are met, such as computational time, number of generations and so on. Let *P(t)* and *C(t)* be parents and offspring (children) in the current generation *t*. The procedures in genetic algorithm can be described as follows (Gen, 1997):

Begin: t=0

Initialize P (t);

Evaluate P (t);

While (not termination condition) do

Recombine P (t) to yield C (t);

(Recombination includes crossover and mutation)

Evaluate C (t);

Select P (t+1) from P (t) and C (t);

t = t +1;

End

End

Complementary to the general procedures discussed above, Figure 4-1 shows the general structures in genetic algorithm (Gen, 1997). Strategies regarding coding of genes, definition of fitness value of an individual, design of crossover and mutation operators, and selection criteria can vary. For example, in Holland's work, encoding is carried out using binary strings. During the past 10 years, real number coding, integer coding and others have appeared (Gen, 1997). Constraints can be handled by rejecting, repairing or a penalty

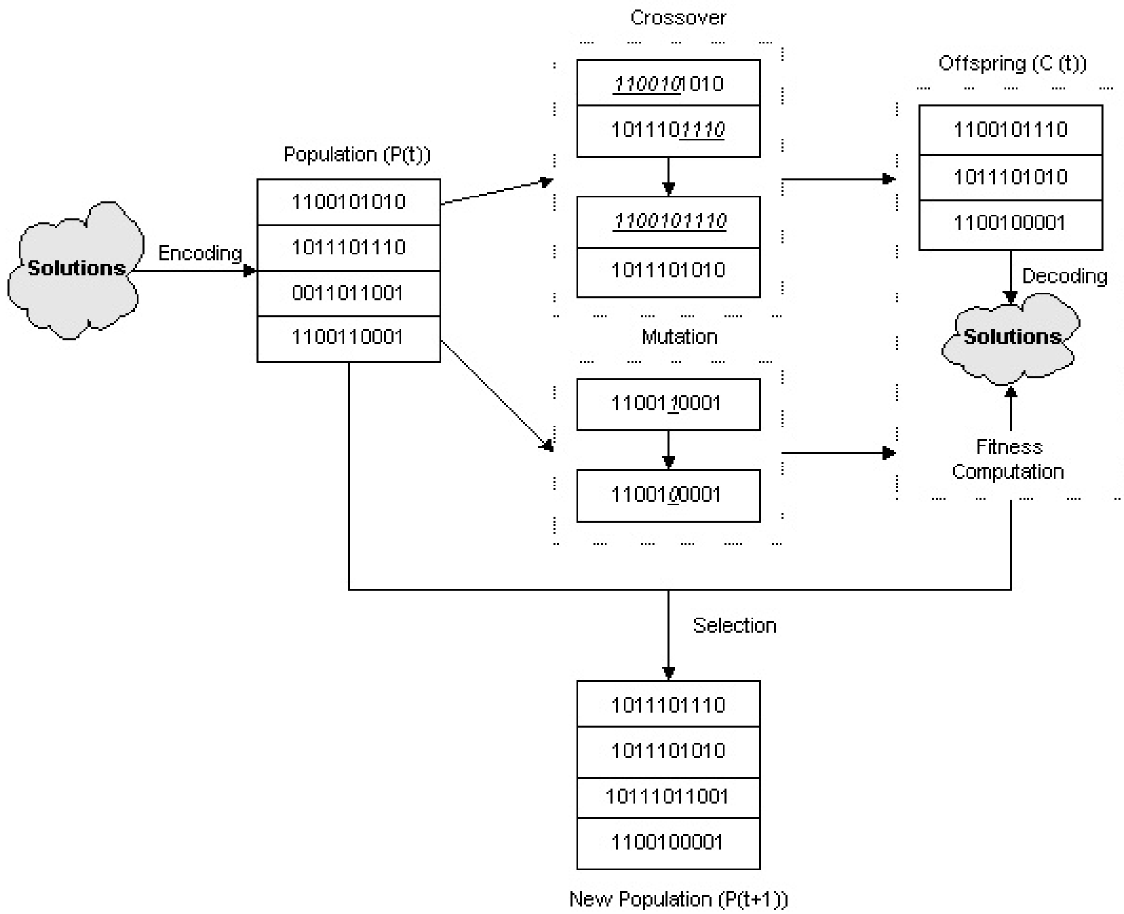


Figure 4-1. The General Structures of Genetic Algorithms (Gen, 1997)

function approach. Selection can be made based on a stochastic mechanism, deterministic mechanism (e.g. truncation selection, elitist selection) or combination of the two mechanisms (e.g. tournament selection) (Gen, 1997). Some common crossover operators are one-point crossover, two-point crossover, cycle crossover and uniform crossover (Pham and Karaboga, 1998). Mutation rate can be fixed or be varying according to fitness value of chromosome (Pham and Karaboga, 1998).

4.2.2 Overview of Evolver

Evolver is a genetic algorithm (GA) based optimization solver developed by Palisade Corporation (Palisade, 1998). It is built as a Microsoft Excel Add-in. The basic steps required to run Evolver are summarized as follows:

(1) Set the objective value for the problems;

(2) Select design variables and setting constraint on design variables;

(3) Specify crossover and mutation operators and rates. Besides the default crossover and mutation operator, Evolver also provides several other operators, such as linear operator and boundary mutations, which can improve the performance and efficiency for certain problems. The default crossover and mutation operator are used throughout the study. The linear operator is also used since there are many linear equations in the IGCC model (Nonlinear equations also exist in the IGCC model). As pointed out in the user's guide of Evolver, the linear operator is designed to solve the problem where optimal solutions lies on the boundary of the search space and is particularly suited for solving linear optimization problem (Palisade, 1998). The default crossover and mutation rates are 0.5 and 0.1, respectively, in Evolver, and users have the option to change them. In this study, the default value for crossover and mutation rate is used.

(4) Set other constraints;

(5) If applicable, specify Excel Macros to run before or after each trial during optimization procedures; This property provides much flexibility in building optimization problems, since optimization problem can be coded in Visual Basic Macros rather than spreadsheet models;

(6) Choose stopping conditions, such as number of trials, running minutes, or change of objective value after a certain number of valid trials is less than some percentage. The last one is the most popular stopping condition (Palisade, 1998). In this study, we use change of objective value after 200 valid trials of less than 1% as stopping condition, which is more conservative than the default value of Evolver (change of objective value after 100 valid trials is less than 1%);

After setting these conditions, one can set the Evolver to start optimizing. When the stopping criteria is met, Evolver stops the optimization process, and reports the best objective function value, and optimal design variables at which the best objective function value is achieved.

4.2.3 Performance of GA in Optimization of Process Models

Before doing optimization under variability and/or uncertainty, two less computationally intensive deterministic optimization cases were carried out to evaluate the performance of Evolver for optimization of process models. The first one involves optimal control of NO_X emissions in an IGCC system, and the second one involves optimal control of SO_2 emissions in an IGCC system.

Case 1: Optimal Control of NO_X Emissions in an IGCC System

In this case study, the performance of Evolver is compared with a mathematical nonlinear programming technique, called Successive Quadratic Programming (SQP). SQP is a nonlinear programming technique and is favored for large scale nonlinear programming problems (Diwekar, *et al*., 1997). The code for SQP is from a Fortran numerical library developed by Visual Numerics Incorporation.

The IGCC system in this case features a gas turbine design with an inlet temperature of 2350 K, pressure ratio of 13.5, and a Selective Catalytic Reduction (SCR) for post-combustion NO_X control. This system corresponds to configuration 2 in the performance and cost model discussed in Chapter 3.

The objective of this problem is to minimize of cost of electricity in mills/kWh, when NO_X emissions are constrained to be less than or equal to 0.3 lb/10^6Btu. It is a nonlinear programming problem, since there are both linear and nonlinear equations in the IGCC model. Design variables are gasifier carbon conversion (CARCNV), gasifier oxygen to carbon ratio (RMOXG2C), gasifier steam to carbon ratio (RSTM2OX), sulfur retained in gasifier bottom ash (XSLCNV), SCR NO_X removal efficiency (SCRAE) and SCR NH_3 slip (XNH3S). Description of the optimization problem is summarized in Table 4-1.

The optimal solutions from Evolver and SQP are summarized in Table 4-2. The optimal cost of electricity is 51.43 mills/kWh found by Evolver, and 51.42 mills/kWh by SQP. The optimal design variable values from the two methods are very close. The optimal points are also similar as shown in Table 4-2. There is a difference regarding the optimal ammonia slip from the two methods. This implies that ammonia slip does not substantially affect the cost of electricity.

This case study suggests that GA can find comparable optimal solutions as the traditional mathematical nonlinear programming method does. However, GA does not require calculation of a gradient, which means that GA can be more robust for certain problems compared with traditional mathematical programming methods, such as SQP. GA can also accommodate discrete design variables. With these advantages, GA is chosen as the optimizer in this study.

Table 4-1. Deterministic Optimization of NO_X Emissions Control in an IGCC System

Objective	Minimization of Cost of Electricity (mills/kWh)
Constraint	NO_X emissions ≤ 0.3 lb/10^6Btu
Design variables	Gasifier Carbon Conversion (CARCNV) Gasifier Oxygen to Carbon Ratio (RMOXG2C) Gasifier Steam to Carbon Ratio (RSTM2OX) Sulfur retained in Gasifier bottom ash (XSLCNV) SCR NOX removal efficiency (SCRAE) SCR NH3 slip (XNH3S)
Constraint on design values	$0.90 \leq$ CARCNV ≤ 0.98 $0.45 \leq$ RMOXG2C ≤ 0.47 $0.445 \leq$ RSTM2OX ≤ 0.455 $0.80 \leq$ XSLCNV ≤ 0.95 $0.50 \leq$ SCRAE ≤ 0.90 $5.0 \leq$ XNH3S ≤ 20.0

Table 4-2. Summary of Optimal Solutions from Evolver and SQP for NO_X Emission Control in an IGCC System

	Evolver	IMSL
Optimization method	Genetic Algorithm (GA)	Successive Quadratic Programming (SQP)
Optimal cost of electricity (year 1989 mills/kWh)	51.43	51.42
Constraint value at optimal point (lb/10^6 Btu)	0.3000	0.3000
Optimal design values	CARCNV=0.980 RMOXG2C=0.450 RSTM2OX=0.455 XSLCNV=0.945 SCRAE=0.517 XNH3S=5	CARCNV=0.980, RMOXG2C=0.450 RSTM2OX=0.455 XSLCNV=0.944 SCRAE=0.515 XNH3S=9.935

Case 2: Optimization of SO_2 Emission Control in an IGCC System

In this case, the SO_2 emissions control in the IGCC system is optimized with Evolver. Results from Evolver are compared with published data. The objective of this case study is to see whether or not optimal solutions can be comparable to those from other researchers.

The IGCC system studied here corresponds to configuration 4 in the performance and cost model discussed in Chapter 3. In this IGCC system, in-bed desulfurization with limestone and external zinc ferrite absorption process are used for SO_2 emissions' control.

Three design variables are chosen, which are in-bed desulfurization efficiency, zinc ferrite absorption cycle time and maximum vessel height to diameter ratio (Diwekar, *et al*., 1992). Description of the problem is summarized in Table 4-3.

The optimal cost of electricity was found to be 55.07 mills/kWh, and the optimal in-bed desulfurization efficiency is 0.804. The optimal zinc ferrite absorption cycle time is 74 hours, and the maximum ratio of the vessel height-to-diameter for the zinc ferrite absorbers is 2.27. Table 4-4 summarizes the optimal cost of electricity and optimal design values. The optimal solution found by Diwekar *et al*. (1992) for the same problem is also given in Table 4-4. The optimal design values are comparable, while the optimal cost of electricity in this study is much higher than that of Diwekar *et al*. (1992). When their design values were implemented into our process model, the cost of electricity was found to be 55.18 mills/kWh, which is higher than the optimal cost of 55.07 mills/kWh found in this study. The difference in optimal cost of electricity can be possibly attributed to differences between cost model parameters used here versus those used by them. For example, if we use \$1.28/10^6Btu for the unit cost of coal instead of \$1.61/10^6Btu, or on average, lower process contingencies and maintenance cost factors by 26%, our optimal cost can be 52.09 mills/kWh.

Though significant difference in optimal cost of electricity exists, the optimal design values are very close especially for the in-bed desulfurization efficiency and the absorption cycle time. The difference in results for the maximum height-to-diameter ratio suggests that this input is not sensitive. These results suggest the feasibility of using GA for optimization of process models.

Table 4-3: Deterministic Optimization of SO_2 Emissions Control in an IGCC System

Objective	Minimization of the cost of electricity;
Constraint:	SO_2 Emission ≤ 0.015 lb/ 10^6Btu;
Design Variables:	In-bed desulfurization efficiency (η_s), Zinc ferrite absorption cycle time (t_a), Maximum ratio of the vessel height to diameter for the zinc ferrite absorbers (Max L/D);
Constraint on the design variables:	$0.8 \leq \eta_s \leq 0.9$; $30 \leq t_a \leq 170$; $2 <$ Max L/D ≤ 4;

Table 4-4: Summary of Optimal solutions for SO_2 Emissions Control in an IGCC System

	Optimal solutions found by Evolver	Optimal solutions from Diwekar et al.(1992)
In-bed desulfurization efficiency η_s	0.804	0.81
Zinc ferrite absorption cycle time t_a (hours)	74.18	84.45
Maximum ratio of the vessel height to diameter for zinc ferrite absorbers (Max L/D)	2.27	4.00
Optimal Cost of the electricity (year 1989 mills/kWh)	55.07	52.09

4.3 Software Organization

Figure 4-2 shows the schematic of the integration of random number files, optimizer, and process model. They are built under the Microsoft Excel environment. Data exchange and running control are achieved by code written in Microsoft Visual Basic.

When doing stochastic optimization, Evolver generates decision values. Design values and random samples are fed into the process model, and the process model is called to generate outputs. This procedure is repeated *N* times if there are *N* realizations for uncertainty. From the *N* model outputs, the probabilistic functional used in stochastic optimization can be approximated, which is then passed to Evolver for generation of new

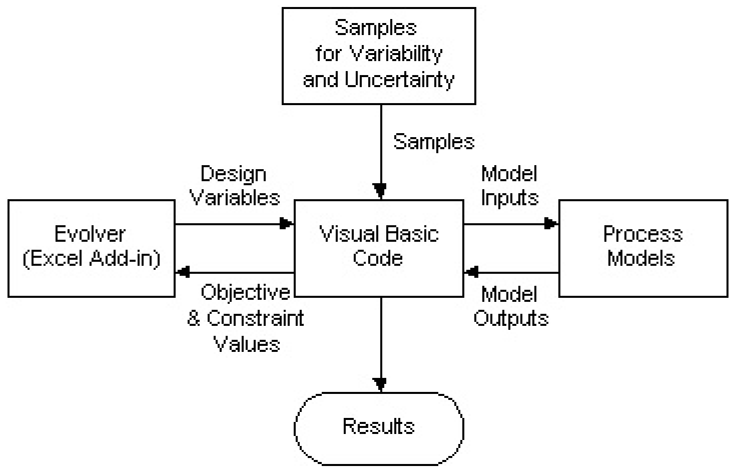


Figure 4-2. Integration of Software for Optimization under Variability and Uncertainty

design values. This process is iterated until optimal solutions are found. A flow diagram for doing stochastic optimization was shown in Figure 2-3 of Chapter 2.

When doing stochastic programming, for each realization of uncertain variables, Evolver is called to find the optimal solutions for this set of random samples. If there are *N* realizations of uncertain variables, *N* optimal solutions will be found. A flow diagram for doing stochastic programming was shown in Figure 2-5 of Chapter 2.

For coupled stochastic optimization and programming technique, stochastic optimization is done for each realization of variability. The output is a probability distribution for optimal solutions from stochastic optimization, which can be used to assess the effect of uncertainties on the stochastic optimization results. The flow diagram for this method was shown in Figure 2-6 of Chapter 2.

For two-dimensional stochastic programming, deterministic programming is done for each combination of samples for variability and uncertainty. The output would be a two-dimensional distribution of optimal solutions. This method enables one to evaluate the effect of both variability and uncertainty in model parameters on optimal solutions. The flow diagram for this method was shown in Figure 2-7 of Chapter 2.

5.0 CASE STUDY OF OPTIMIZATION UNDER VARIABILITY AND UNCERTAINTY

This chapter presents the results from three case studies based on minimizing levelized cost subject to a NO_X emissions constraint. These three cases are:

(1) Stochastic optimization and stochastic programming when only variability in model inputs is considered;

(2) Stochastic optimization and stochastic programming when only uncertainty in model inputs is considered;

(3) Coupled stochastic optimization and programming, and two-dimensional stochastic programming methods when both variability and uncertainty in model inputs are considered.

The IGCC system features a gas turbine with pressure ratio of 13.5 and turbine inlet temperature of 2300 K, and a Selective Catalytic Reduction (SCR) process for post combustion NO_X emissions control. The system corresponds to Configuration 3 in the IGCC model discussed in Chapter 3 and given in Table 3-1. A summary of key characteristics of the plant, such as net electricity generated, efficiency and so on is given in Table 5-1, when all model inputs are at default values. Optimization under variability and uncertainty with regard to Configuration 2 in the IGCC model was also done. The results are very similar to those of Configuration 3, and are summarized in Appendix B.

To achieve a cost effective control of NO_X emissions, seven variables in the system were identified and chosen as design variables. These variables include: gasifier oxygen to carbon ratio (RMOXG2C), gasifier steam to carbon ratio (RSTM2OX), sulfur retained in the gasifier bottom ash (XSLCNV), SCR NO_X removal efficiency (SCRAE), SCR ammonia slip

Table 5-1. A Summary of Key Characteristics of the Studied IGCC System

Name	Values
Net Electricity (10^6Watt)	725.08
Heat Rate (Btu/kW, HHV basis)	8348.58
Efficiency (fraction, HHV basis)	0.4091
Capital Cost ($/kW)	1693.58
Fixed Operating Cost* ($/kW-year)	55.47
Variable Operating Cost* (mills/kWh)	21.2
Cost of Electricity* (mills/kWh)	61.70
Coal Input (lb/kWh)	0.7422
CO_2 Emissions (lb/kWh)	1.7225
SO_2 Emissions (lb/10^6Btu)	0.0133
NO_X Emissions (lb/10^6Btu)	0.1223

*: Dollar values based on January, 2002.

(XNH3S), SCR catalyst layer replacement interval (REPHRS) and capacity factor (CF). RMOXG2C, RSTM2OX, XSLCNV are important design variables with regard to the gasifer, while SCRAE, XNH3S and REPHRS are variables directly connected with performance and cost of SCR process. The adjustable range and default values of these variables are given in Table 5-2.

5.1 Optimization Considering Variability in Model Inputs

In this part, stochastic optimization and stochastic programming are conducted when variability in model inputs is considered. As discussed in Section 3.3, twenty six variables were identified with variability, and probabilistic distributions were developed to characterize the variability for these variables, which are shown in Table 3-5. For each of these variables, 100 random samples are generated through AuvTool. The same random samples are used for both stochastic optimization and stochastic programming, and thus comparison between the results of two methods will not be interfered with differences in the sequence of random numbers. For those variables with only uncertainty, default point estimates were used, which are shown in Table 3-3.

Table 5-2. Description of Design Variables and Adjustable Range

Design variables	Description	Default Value	Adjustable Range
RMOXG2C	Gasifier oxygen to carbon ratio	0.46	0.45 ~ 0.47
RSTM2OX	Gasifier steam to carbon ratio	0.45	0.445 ~ 0.455
XSLCNV	Sulfur retained in the gasifier bottom ash	0.90	0.80 ~ 0.95
SCRAE	SCR NO_X removal efficiency	0.80	0.50 ~ 0.90
XNH3S	SCR ammonia slip (ppm)	10	5.0 ~ 20.0
RSPHRS	SCR catalyst layer replacement interval (hour)	11390	5000 ~ 25000
CF	Capacity factor	0.65	0.5 ~ 0.9

5.1.1 Results from Stochastic Optimization

The objective of stochastic optimization is to minimize the expected value of cost of electricity when NO_X emissions are constrained. Different statistics of NO_X emissions can be constrained, such as the expected value, 90th percentile, or 95th percentile. In the following two cases, the expected value of NO_X emissions is constrained in the first case, and the 90th percentile of NO_X emissions is constrained in the second case.

Case 1: Expected Value of NO_X Emissions is Constrained

In this case, the expected value of NO_X emissions is constrained to be less than or equal to a particular value. The objective is to minimize expected cost of electricity. Design variables were discussed and are given in Table 5-2.

Figure 5-1 shows the optimal expected cost of electricity when the expected value of NO_X emissions is constrained to be less than or equal to 0.3 lb/10^{6}Btu, 0.2 lb/10^{6}Btu and 0.1 lb/10^{6}Btu, respectively. When the expected NO_X emissions are constrained to be not greater than 0.3 lb/10^{6}Btu, the optimal expected cost of electricity is 50.34 mills/kWh. As expected, when expected NO_X emissions are constrained to be not greater than 0.2 lb/10^{6}Btu, the optimal expected cost of electricity goes up. The expected cost of electricity in this case is 50.45 mills/kWh, and the required SCR removal efficiency is 60%. When the expected NO_X

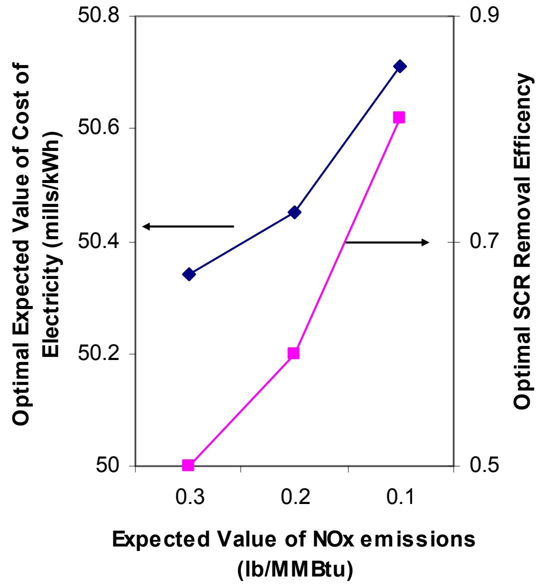


Figure 5-1. Optimal Expected Cost of Electricity from Stochastic Optimization Considering Variability in Model Inputs when Expected Value of NO_X Emissions is Constrained

emissions constraint becomes 0.1 lb/10^6Btu, the optimal expected cost of electricity increases to 50.71 mills/kWh and the required SCR removal efficiency is 81%. To place these results in context, for a 730,000 kW power plant with an annual capacity factor of 0.65, a difference in cost of electricity of 0.37 mills/kWh, based upon comparing the results for the NO_X constraints of 0.3 and 0.1 lb/10^6Btu, is $1.54 millions per year. Detailed optimal solutions for all the three constraint levels are summarized in Table 5-3. As shown in Table 5-3, the optimal values for "Gasifier oxygen to carbon ratio" and "SCR ammonia slip" are at their lower bounds. However, optimal values for "Sulfur retained in the gasifier bottom ash", "Gasifier steam to carbon ratio", "SCR catalyst layer replacement interval" and "Capacity factor" are at upper bounds. Optimal values for "SCR removal efficiency" vary as the expected values of NO_X emissions are constrained by different levels.

Table 5-3. Optimal Solutions from Stochastic Optimization Considering Variability in Model Inputs when Expected Value of NO_X Emissions is Constrained

	Level 1	Level 2	Level 3
Expected value of NO_X Emissions (lb/10^6 Btu)	≤ 0.3	≤ 0.2	≤ 0.1
Minimum expected cost of electricity (mills/kWh)	50.34	50.45	50.71
Optimal gasifier oxygen to carbon ratio	0.45	0.45	0.45
Optimal gasifier steam to carbon ratio	0.455	0.455	0.455
Optimal sulfur retained in the gasifier bottom ash	0.95	0.95	0.95
Optimal SCR NO_X removal efficiency	0.5	0.60	0.81
Optimal SCR ammonia slip	5	5	5
Optimal SCR catalyst layer replacement interval (hour)	25000	25000	25000
Optimal capacity factor	0.9	0.9	0.9

The optimal values for the design variables are reasonable. To evaluate the optimized results, the sensitivity of cost of electricity to each design variable is done while keeping other design variables at default values (see Table 5-2 for default values of design variables; Table 3-3 for default values of uncertain variables; and Table 3-4 for default values of variables with both variability and uncertainty). Figure 5-2 to Figure 5-8 shows the sensitivity of cost of electricity to each design variable. Figure 5-2 shows that cost of electricity will increase approximately linearly with the increase of gasifier oxygen to carbon ratio (RMOXG2C). High RMOXG2C value increases the net electricity of the system, but it also increases the capital and operating cost of the system. Overall, high RMOXG2C results in high cost of electricity. Thus, the optimal RMOXG2C is at the lower bound.

Figure 5-3 shows that the cost of electricity is not sensitive to gasifier steam to carbon ratio (RSTM2OX). The increase of RSTM2OX results in a slight decrease of SCR NO_X load, which consequently decreases a bit of the operating cost. However, the effect of RSTM2OX on the overall cost of electricity is very small. If RSTM2OX is 0.455, the cost of electricity is

61.69 mills/kWh, which is 0.01 mills/kWh lower than that when RSTM2OX is at 0.445. The Optimal RSTM2OX is at the high bound.

Figure 5-4 shows that an increase of sulfur retained in the gasifier bottom ash (XSLCNV) can generally decrease the cost of electricity. High values of XSLCNV decrease both the steam turbine output and auxiliary load. The overall net electricity is increased as XSLCNV increases. Thus, high XSLCNV is favored for the minimization of cost of electricity.

Figure 5-5 shows that cost of electricity increases linearly with an increase of the SCR NO_X removal efficiency (SCRAE). Thus, SCRAE should be as low as possible for the optimal cost of electricity. However, SCRAE is also constrained by NO_X emissions. When constraint on expected NO_X emissions changes from 0.3 lb/10^6Btu to 0.2 lb/10^6Btu, the required SCR removal efficiency increases from 0.50 to 0.60.

Figure 5-6 shows the sensitivity of cost of electricity to SCR ammonia slip (XNH3S). The cost of electricity is not sensitive to XNH3S. The cost of electricity only increases by 0.01 mills/kWh when XNH3S is increased from 5 to 20ppm. Detailed analysis indicates that an increase of XNH3S causes an increase in ammonia consumptions, which increases the cost of electricity. The optimal XNH3S is at its lower bound.

Figure 5-7 shows that capacity factor (CF) can have a significant nonlinear impact on the cost of electricity. Cost of electricity drops from 73 mills/kWh when CF is 0.5 to about 50 mills/kWh when CF is 0.9. The maximum CF increases the utilization of the system, and thus lowers the cost of electricity. The optimal capacity factor is at the high bound.

Figure 5-8 shows the sensitivity of cost of electricity to SCR catalyst layer replacement interval (REPHRS). When REPHRS increases, the capital cost of SCR process

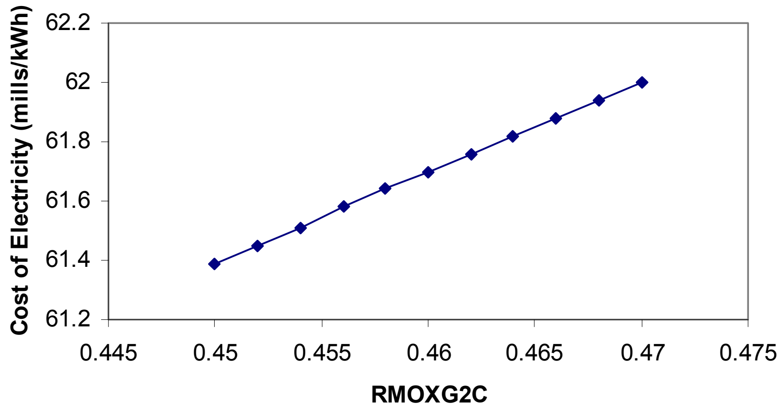


Figure 5-2. Sensitivity of Cost of Electricity to Gasifier Oxygen to Carbon Ratio (RMOXG2C) when Other Design Variables are at Default Values

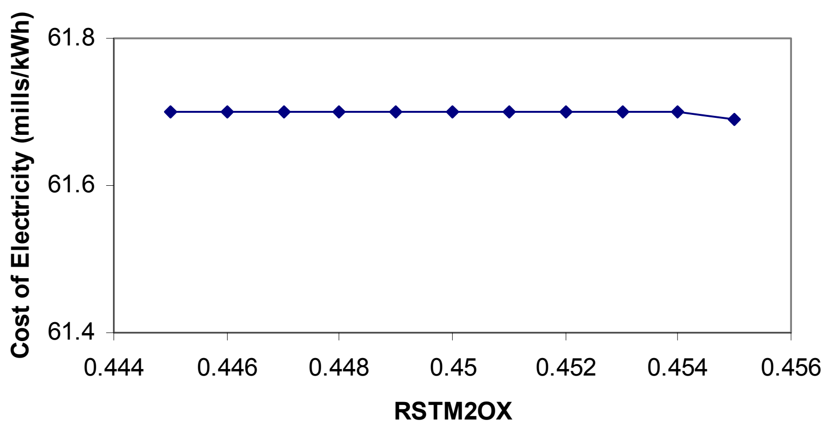


Figure 5-3. Sensitivity of Cost of Electricity to Gasifier Steam to Carbon Ratio (RSTM2OX) when Other Design Variables are at Default Values

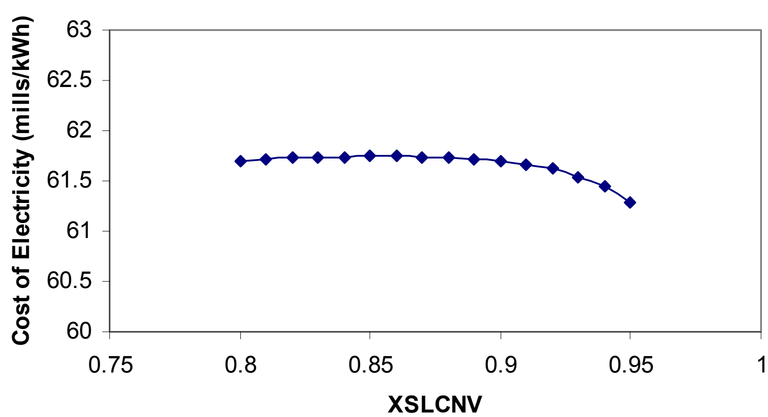


Figure 5-4. Sensitivity of Cost of Electricity to Sulfur Retained in the Gasifier Bottom Ash (XSLCNV) when Other Design Variables are at Default Values

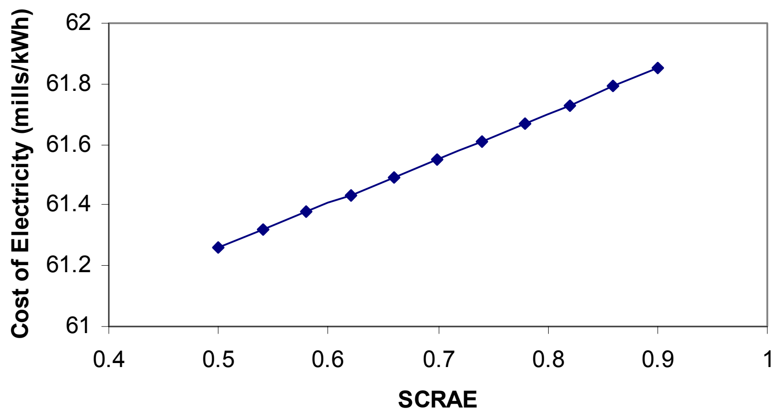


Figure 5-5. Sensitivity of Cost of Electricity to SCR NO_X Removal Efficiency (SCRAE) when Other Design Variables are at Default Value

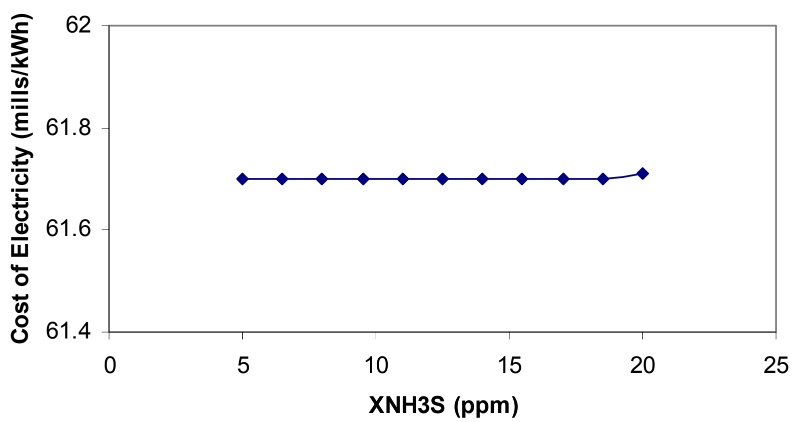


Figure 5-6. Sensitivity of Cost of Electricity to SCR Ammonia Slip (XNH3S) when Other Design Variables are at Default Values

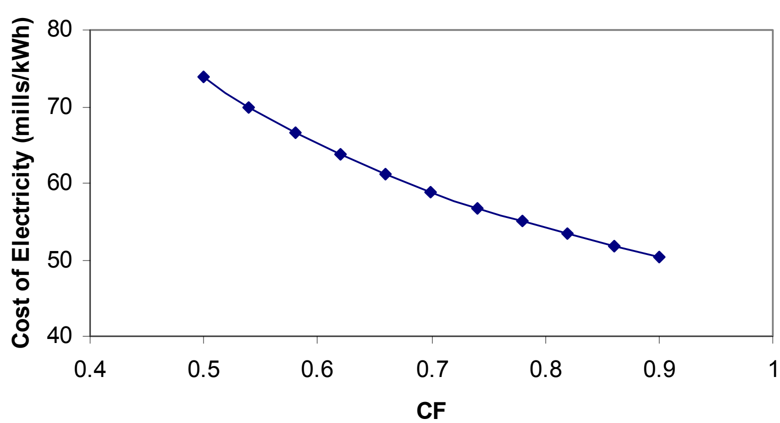


Figure 5-7. Sensitivity of Cost of Electricity to Capacity Factor (CF) when Other Design Variables are at Default Values

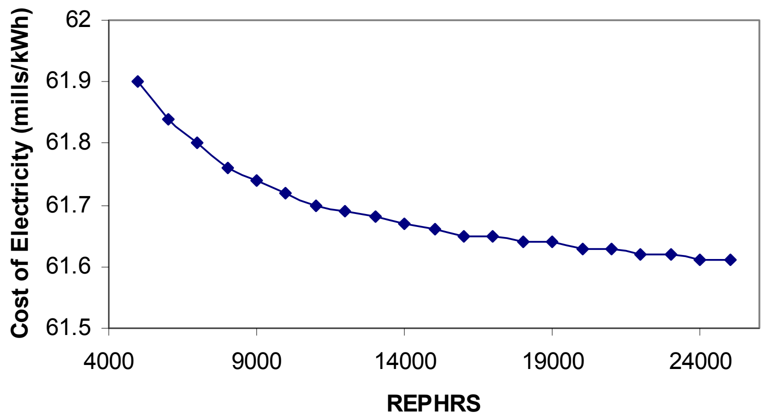


Figure 5-8. Sensitivity of Cost of Electricity to SCR Catalyst Layer Replacement Interval (REPHRS) when Other Design Variables are at Default Value

area will increase, but the operating cost will decrease. Overall, high values of REPHRS decrease the cost of electricity. Thus, the optimal REPHRS is at the high bound.

Case 2: 90th Percentile of NO_X Emissions is Constrained

In this case, the 90th percentile of NO_X emissions is constrained by a particular value. The objective value and design variables remain the same as for Case 1.

Figure 5-9 shows the optimal expected value of cost of electricity when the 90th percentile of NO_X emissions is constrained by 0.3 lb/10^6Btu, 0.2 lb/10^6Btu and 0.1 lb/10^6Btu, respectively. The general trend of the optimal expected cost of electricity is similar to the Case 1, where the expected value of NO_X emissions is constrained. However, the optimal expected cost of electricity in this case is higher than that of Case 1. For example, when expected NO_X emissions are constrained by 0.2 lb/10^6Btu, the optimal expected cost of electricity is 50.45 mills/kWh; while the optimal expected cost of electricity is 50.55 mills/kWh, when the 90th percentile of NO_X emissions is constrained by 0.2 lb/10^6Btu. Optimal design values are summarized in Table 5-4.

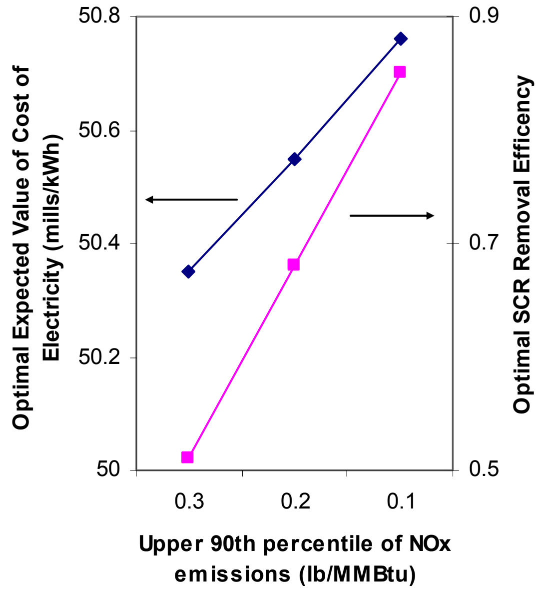


Figure 5-9. Optimal Expected Value of Cost of Electricity from Stochastic Optimization Considering Variability in Model Inputs when 90th Percentile of NO_X Emissions is Constrained

Table 5-4. Optimal Solutions from Stochastic Optimization Considering Variability in Model Inputs when 90th Percentile of NO_X Emissions is Constrained

	Level 1	Level 2	Level 3
Constraint on NO_X Emission ($lb/10^6$ Btu)	90 percentile of NO_X emissions $\leqslant 0.3$	90 percentile of NO_X emissions $\leqslant 0.2$	90 percentile of NO_X emissions $\leqslant 0.1$
Minimum expected cost of electricity	50.35	50.55	50.76
Gasifier Oxygen to Carbon Ratio	0.45	0.45	0.45
Gasifier Steam to Carbon Ratio	0.455	0.455	0.455
Sulfur retained in the gasifier bottom ash	0.95	0.95	0.95
SCR NO_X Removal Efficiency	0.51	0.68	0.85
SCR ammonia slip	5	5	5
Plant Capacity Factor	0.9	0.9	0.9
SCR Replacement Interval	25000	25000	25000

Except for the SCR removal efficiency, all other variables in these cases have the same optimal values as the cases in which expected NO_X emissions are constrained.

In addition to the two cases discussed above, the optimal expected cost of electricity is also evaluated when different statistics (e.g. expected value, 90th percentile, 95th percentile, 97th percentile, and 99th percentile) of NO_X are constrained to be less than or equal to 0.2 lb/10^6Btu. Table 5-5 shows the optimal solutions under these five constraints. As the constraint on NO_X emissions becomes stricter, the SCR removal efficiency increases, and so does the optimal expected cost of electricity. For example, the optimal expected cost of electricity is 50.62 mills/kWh when the 99th percentile of NO_X emissions is constrained, which is 0.17 mills/kWh higher than the base case, in which expected value of NO_X emissions is constrained.

Table 5-5. Optimal Solutions from Stochastic Optimization Considering Variability in Model Inputs when Different Statistics of NO_X Emissions are Constrained to be less than or equal to 0.2 lb/ 10^6Btu

	Level 1	Level 2	Level 3	Level 4	Level 5
Constraint (Unit of NO_X emissions is lb/10^6Btu)	Expected value of NO_X emissions ≤ 0.2	Probability (NO_X emissions $\leq 0.2) \geq 0.9$	Probability (NO_X emissions $\leq 0.2) \geq 0.95$	Probability (NO_X emissions $\leq 0.2) \geq 0.97$	Probability (NO_X emissions $\leq 0.2) \geq 0.99$
Optimal expected cost of electricity (mills/kWh)	50.45	50.55	50.59	50.61	50.62
Gasifier Oxygen to Carbon Ratio	0.45	0.45	0.45	0.45	0.45
Gasifier Steam to Carbon Ratio	0.455	0.455	0.455	0.455	0.455
Sulfur retained in the gasifier bottom ash	0.95	0.95	0.95	0.95	0.95
SCR NO_X Removal Efficiency	0.60	0.68	0.71	0.73	0.74
SCR ammonia slip	5	5	5	5	5
Plant Capacity Factor	0.9	0.9	0.9	0.9	0.9
SCR Replacement Interval	25000	25000	25000	25000	25000

5.1.2 Results from Stochastic Programming

In contrast to stochastic optimization, stochastic programming involves deterministic optimization for each random sample. Stochastic programming generates 100 optimal solutions if 100 random numbers are sampled for variability. This section summarizes results from stochastic programming for variability only. At each stage of stochastic programming, objective is to minimize of the cost of electricity (mills/kWh).

Figure 5-10 shows the cumulative probability distribution of optimal cost of electricity when NO_X emissions are constrained to less than or equal to 0.2 lb/10^6Btu. The mean optimal cost of electricity is around 50.45 mills/kWh. In specific situations, the optimal cost of electricity can go up to 53.15 mills/kWh and the overall range is 45.92 to 53.15 mills/kWh. This suggests that variability can significantly affect the optimal cost of the system. The cumulative probability distribution of optimal SCR removal efficiency is given in Figure 5-11. The average optimal SCR removal efficiency is 59%. However, given variability in model inputs, the optimal SCR removal efficiencies vary from 50 to 74 percent.

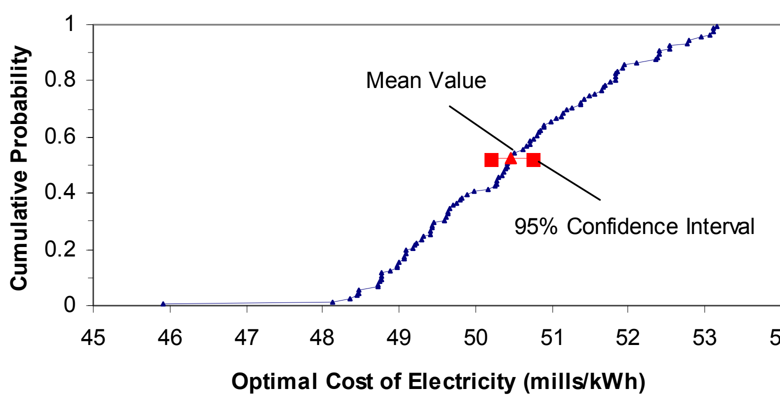


Figure 5-10. Cumulative Probability of Optimal Cost of Electricity from Stochastic Programming Considering Variability in Model Inputs when NO_X Emissions are Constrained to Less Than or Equal to 0.2 lb/10^6Btu

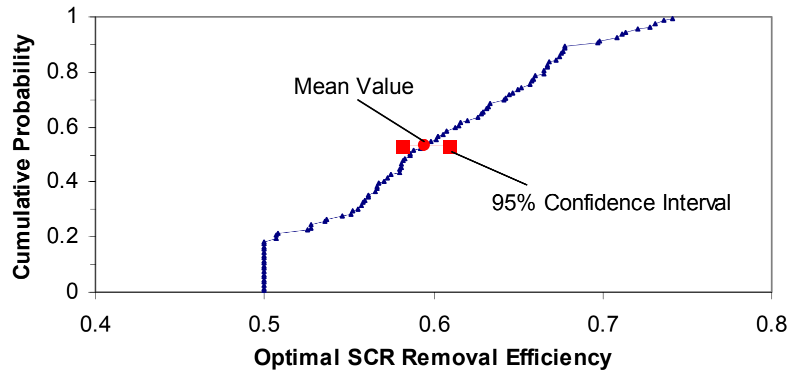


Figure 5-11. Cumulative Probability Distribution for Optimal SCR Removal Efficiency in Stochastic Programming Considering Variability in Model Inputs when NO_X Emissions are Constrained to be Less than or Equal to 0.2 lb/10^6Btu

Stochastic programming was also conducted when NO_X emissions were constrained to be less than or equal to 0.1 lb/10^6Btu, and 0.3 lb/10^6Btu, respectively. Table 5-6 summarizes optimal solutions from stochastic programming for three NO_X emissions constraints. The average value and 95% variability range for the optimal cost of electricity and optimal design values are given in Table 5-6. For all three levels, the 95% range of optimal costs of electricity vary from -4% to 5% compared with the mean value, on a relative basis.

Optimal values for gasifier oxygen to carbon ratio (RMOXG2C), sulfur retained in the gasifier bottom ash (XSLCNV) and capacity factor (CF) do not change during the 100 realizations of variability. However, optimal values for SCR ammonia slip (XNH3S), gasifier steam to carbon ratio (RSTM2OX), SCR removal efficiency (SCRAE) and SCR catalyst layer replacement interval (REPHRS) vary. In two of these cases, relative ranges of variation are small. For example, RSTM2OX and REPHRS vary only by a small percentage of their mean values and change little for the three emissions levels. Ammonia slip appears to vary

Table 5-6. Minimization of Cost of Electricity using Stochastic Programming when Considering only Variability in Model Inputs

	Level 1	Level 2	Level 3
Constraint on NO_X Emissions ($lb/10^6 Btu$)	NO_X emissions ⩽0.3	NO_X emissions ⩽0.2	NO_X emissions ⩽0.1
Mean Value of the Optimal cost of electricity (mills/kWh)	50.35	50.45	50.71
95% range of optimal cost of electricity (mills/kWh)	48.45 ~ 52.96	48.59 ~ 53.09	45.84 ~ 53.34
Mean value of optimal RMOXG2C	0.45	0.45	0.45
95% range of optimal RMOXG2C	0.45 ~ 0.45	0.45 ~ 0.45	0.45 ~ 0.45
Mean value of optimal RSTM2OX	0.454	0.453	0.453
95% range of optimal RSTM2OX	0.452 ~ 0.455	0.450 ~ 0.455	0.451 ~ 0.455
Mean value of optimal XSLCNV	0.95	0.95	0.95
95% range of optimal XSLCNV	0.95 ~ 0.95	0.95 ~ 0.95	0.95 ~ 0.95
Mean value of optimal SCRAE	0.51	0.59	0.80
95% range of optimal SCRAE	0.5 ~ 0.59	0.5 ~ 0.73	0.72 ~ 0.87
Mean value of optimal XNH3S	6.2	9.4	10.1
95% range of optimal XNH3S	5 ~ 12.1	5 ~ 18.0	5 ~ 16.4
Mean value of optimal CF	0.9	0.9	0.9
95% range of optimal CF	0.9 ~ 0.9	0.9 ~ 0.9	0.9 ~ 0.9
Mean value of optimal REPHRS	24849	24894	24702
95% range of optimal REPHRS	24070 ~ 25000	24356 ~ 25000	24104 ~ 25000

but was previously shown to be an insensitive input. SCRAE varies substantially and is a sensitive input. Two model inputs, the fraction of NH_3 converted to NO_X in the gas turbine (XXNH3) and the fraction of coal bound nitrogen converted NH_3 (XXCRN), are assumed to have variability. These two inputs impact the NO_X concentrations in the flue gas upstream of the SCR process. Thus optimal SCR NO_X removal efficiency is expected to vary in response to the variations in XXNH3 and XXCRN to meet the constraint on NO_X emissions. Figure 5-12 and Figure 5-13 shows the variations of optimal SCR NO_X removal efficiency with the variations of XXCRN and XXNH3 (for the case of NO_X emissions ≤ 0.2 lb/10^6Btu). There is a clear correlation between the optimal SCR NO_X removal efficiency and XXCRN (Sample correlation coefficient is 0.80). Dependence of optimal SCR NO_X removal efficiency on XXNH3 is not as strong as on XXCRN, though the correlation is still statistically significant on a 95% level of confidence (Sample correlation coefficient is 0.34).

5.1.3 Comparison between Results from Stochastic Optimization and Stochastic Programming

Comparison between optimal solutions from stochastic optimization and stochastic programming enables evaluation of the expected value of perfect information (EVPI). EVPI is the difference between the expected loss (or cost) of optimal management decision based on the results of uncertainty analysis and the expected loss of the optimal management decision if all uncertainty were eliminated in one or all uncertainty quantities. In actual application, EVPI is an upper bound for the expected value of efforts to reduce uncertainty, and as such, provides the ultimate bound on what should be spent on research and data collection efforts (Dakins, 1999). EVPI is calculated by Equation (5-1) (Morgan and Henrion, 1990).

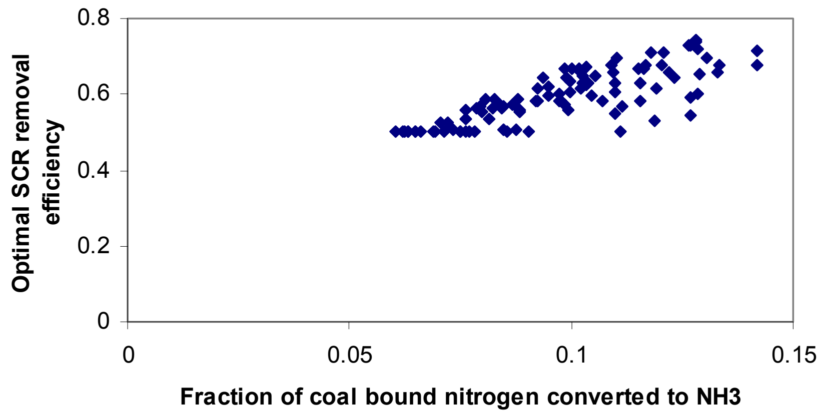


Figure 5-12. Dependence of Optimal SCR Removal Efficiency on the Fraction of Coal Bound Nitrogen Converted to NH3

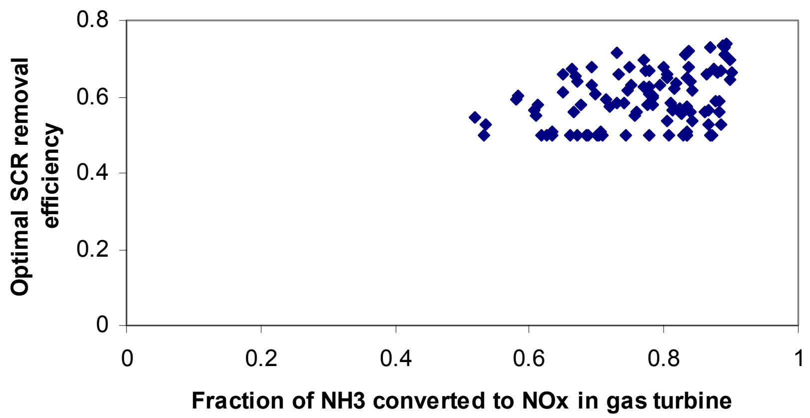


Figure 5-13. Dependence of Optimal SCR Removal Efficiency on the Fraction of NH3 Converted to NO_X in the gas turbine

$$EVPI \equiv Min_d E[L(d,x)] - E[Min_d L(d,x)] \qquad (5\text{-}1)$$

Where, d is the decision chosen from decision space,

x is an uncertain empirical variables,

$L(d,x)$ is the loss function of decision d and state x,

$E[L(d,x)] = \int_X L(d,x) f(x) dx$ is prior expectation over x of the loss for decision d, *f(x)* is probability density on x,

$Min_d L(d, x)$ is the decision that minimize loss given perfect information of x.

The first term in Equation (5-1) is the minimized expected loss. The second term in Equation (5-1) is calculated by determining the minimized loss for the each iteration of the Monte Carlo simulation, when a probabilistic analysis has been carried out using Monte Carlo technique (Dakins, 1999). EVPI has been widely applied in practical problems, such as environmental remediation (Dakins *et al.*, 1994), global warming (Nordhaus and Popp, 1997; Gjerde *et al.*, 1998) and operational planning (Ierapetritou *et al.*, 1995).

EVPI is applied for problems with uncertainty. However, only variability in model inputs is considered here. Under this condition, we apply this concept as the difference in cost of two decision strategies: One is a single optimal control strategy (a single set of decision variables) accommodating variability in model inputs; and the other one is the strategy in which decision values vary with the variations in variables with variability. In this way, EVPI provides the benefit of dynamically adjusting decision variables for optimal control. It can be calculated as the difference between the optimal expected cost of electricity from stochastic optimization and the average optimal cost of electricity from stochastic programming. The loss function is the cost of electricity in this case.

Table 5-7 summarizes the comparisons of stochastic optimization and stochastic programming results under certain conditions. The stochastic programming result shown in the table comes from the case study when NO_X emissions are constrained to be less than or equal to 0.2 lb/10^6Btu. Four stochastic optimization results are shown, in which expected value of NO_X emissions, 90^{th} percentile of NO_X emissions, 95^{th} percentile of NO_X emissions,

Table 5-7. Comparison of Stochastic Optimization and Stochastic Programming Results when Considering Variability in Model Inputs

	Level 1	Level 2	Level 3	Level 4
Optimal value of stochastic optimization				
Constraint ($lb/10^6Btu$)	Expected NO_X emissions ≤ 0.2	Probability (NO_X emissions $\leq 0.2) \geq 0.9$	Probability (NO_X emissions $\leq 0.2) \geq 0.95$	Probability (NO_X emissions $\leq 0.2) \geq 0.99$
Expected Cost of Electricity (mills/kWh)	50.45	50.55	50.59	50.62
SCR Removal Efficiency	0.60	0.68	0.71	0.74
Average optimal value of stochastic programming				
Constraint ($lb/10^6Btu$)	NO_X emissions ≤ 0.2	NO_X emissions ≤ 0.2	NO_X emissions ≤ 0.2	NO_X emissions ≤ 0.2
Cost of Electricity (mills/kWh)	50.45	50.45	50.45	50.45
SCR Removal Efficiency	0.60	0.60	0.60	0.60
Expected Value of Perfect Information (EVPI)				
mills/kWh	0.00	0.10	0.14	0.17
10^6\$/year	0.00	0.60	0.84	1.02

and 99th percentile of NO_X emissions are constrained to be not greater than 0.2 $lb/10^6Btu$, respectively. Choosing to compare these four stochastic optimization results with stochastic programming results are subjective, and it is up to decision makers regarding the reliability of stochastic optimization design (e.g. which statistics of emissions are used as constraint). In stochastic programming, as NO_X emissions are constrained by 0.2 $lb/10^6Btu$, the average optimal cost of electricity is 50.45 mills/kWh. In stochastic optimization, when 90th percentile of NO_X emissions is constrained, the optimal expected cost of electricity is 50.55 mills/kWh, which is 0.10 mills/kWh higher than the average optimal values from stochastic programming. As the net electricity of the system is about 730,000 kW and the capacity is 0.9, 0.10 mills/kWh equals to \$0.6 millions per year. This will be the benefit if the exact values of variables with variability at specific time are known, and decision variables are adjusted according to the exact values of the variables with variability. In stochastic optimization, the required SCR removal efficiency is 0.68, while in stochastic programming, the average required SCR removal efficiency is 0.60. As shown in Figure 5-8, cost of electricity increases as SCR removal efficiency increases. This explains the difference between optimal expected value from stochastic optimization and average optimal value from stochastic programming. When 95th percentile of NO_X emissions is constrained by 0.2 lb/10^6Btu in stochastic optimization, the optimal expected cost of electricity is 50.59 mills/kWh, which is 0.14 mills/kWh higher than average optimal values from stochastic programming. When 99th percentile of NO_X emissions is constrained by 0.2 lb/10^6Btu in stochastic optimization, the optimal expected cost of electricity is 50.62 mills/kWh, which is 0.17 mills/kWh higher than average optimal cost of electricity from stochastic programming.

5.2 Optimization Considering Uncertainty in Model Inputs

In Section 5.1, optimization was conducted when only variability in model inputs is considered. In this section, optimization considering uncertainty in model inputs is explored for the same IGCC system as in Section 5.1. As discussed in Chapter 3, 27 model inputs were identified as uncertain variables. Probabilistic distributions have been developed to characterize the uncertainty, and are given in Table 3-3. For each uncertain input, 100 random samples were generated using AuvTool, and were used in both stochastic optimization and stochastic programming. For the other 26 variables with both variability and uncertainty, the uncertainty associated with the mean of these variables is considered. This uncertainty was which have been characterized with probability distributions as given in

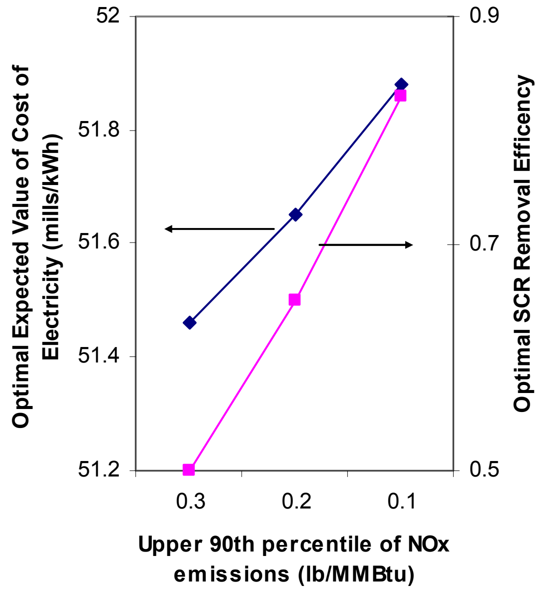


Figure 5-14. Optimal Expected Cost of Electricity from Stochastic Optimization Considering Uncertainty in Model Inputs when the 90th Percentile of NO_X Emissions is Constrained

Table 3-6. Similarly, 100 random samples are generated through AuvTool for each variable of these 26 inputs to represent uncertainty in the mean value.

5.2.1 Results from Stochastic Optimization

The objective of stochastic optimization over uncertainty is to minimize the expected cost of electricity when the 90th percentile of NO_X emissions is constrained. This can be viewed as a chance constrained optimization problem. Other statistics of NO_X emissions, such as expected values, or other percentiles, can also be used as constraint. Here 90th percentile of NO_X emissions is chosen.

Figure 5-14 shows the optimal expected value of cost of electricity when the 90th percentile of NO_X emissions is constrained to be less than or equal to 0.3 lb/10^6Btu, 0.2 lb/10^6Btu and 0.1 lb/10^6Btu, respectively. As the constraint on NO_X emissions becomes stricter, the SCR removal efficiency needs to be increased, which consequently increases the

Table 5-8. Optimal Solutions from Stochastic Optimization Considering Uncertainty in Model Inputs when 90th Percentile of NO_X Emissions is Constrained

	Level 1	Level 2	Level 3
Constraint on NO_X Emission ($lb/10^6$ Btu)	90th percentile of NO_X emissions $\leqslant$0.3	90th percentile of NO_X emissions $\leqslant$0.2	90th percentile of NO_X emissions $\leqslant$0.1
Minimum expected cost of electricity (mills/kWh)	51.46	51.65	51.88
Gasifier Oxygen to Carbon Ratio	0.45	0.45	0.45
Gasifier Steam to Carbon Ratio	0.455	0.455	0.455
Sulfur retained in the gasifier bottom ash	0.95	0.95	0.95
SCR NO_X Removal Efficiency	0.50	0.65	0.83
SCR ammonia slip (ppm)	5	5	5
Plant Capacity Factor	0.9	0.9	0.9
SCR Replacement Interval	25000	25000	25000

expected cost of electricity. The trend of expected cost of electricity with respect to change of the NO_X emissions constraint is similar to the case when variability in model inputs is considered. The optimal design values are summarized in Table 5-8. For the three levels shown in the table, optimal values of SCR removal efficiency are different, while all other design variables have same optimal values. The optimal values are consistent with the results when variability in model inputs is considered, which are shown in Table 5-3.

5.2.2 Results from Stochastic Programming

Stochastic programming involves deterministic optimization for each iteration of random samples. At each iteration, the objective is to minimize the cost of electricity (mills/kWh), given the deterministic constraint on the NO_X emissions.

Figure 5-15 shows the cumulative probability distribution of the optimal cost of electricity when NO_X emissions are constrained to be less than or equal to 0.2 $lb/10^6$Btu. The

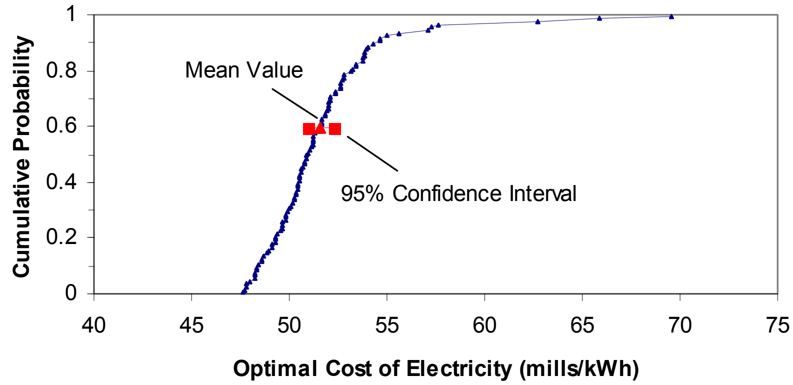


Figure 5-15. Cumulative Probability of Optimal Cost of Electricity from Stochastic Programming Considering Uncertainty in Model Inputs when NO_X Emissions is Constrained to be less than or equal to 0.2 lb/10^6Btu

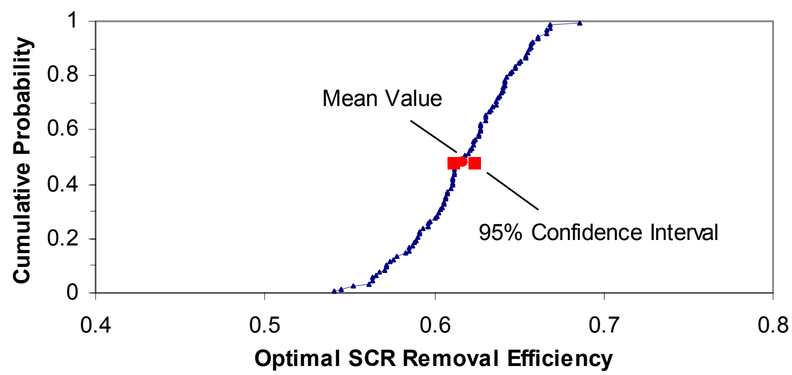


Figure 5-16. Cumulative Probability of Optimal SCR Removal Efficiency from Stochastic Programming Considering Uncertainty in Model Inputs when NO_X Emissions is Constrained to be less than or equal to 0.2 lb/10^6Btu

mean optimal cost of electricity is 51.61 mills/kWh. However, for some uncertainty realizations, the optimal cost of electricity is more than 60 mills/kWh. This suggests that the uncertainty in model inputs significantly impacts the optimal cost of the system. The cumulative probability distribution of the SCR removal efficiency is given in Figure 5-16. The optimal SCR removal efficiency varies from 53% to 70%. Figure 5-17 and Figure 5-18 shows the variations of optimal SCR NO_X removal efficiency with the variations of XXCRN and XXNH3 (for the case of NOX emissions $\leq$ 0.2lb/10^6Btu). There is a clear correlation

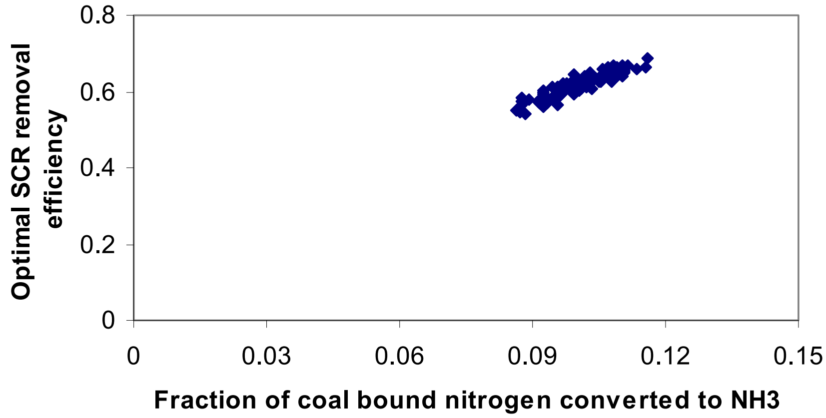


Figure 5-17. Dependence of Optimal SCR Removal Efficiency on the Fraction of Coal Bound Nitrogen Converted to NH3

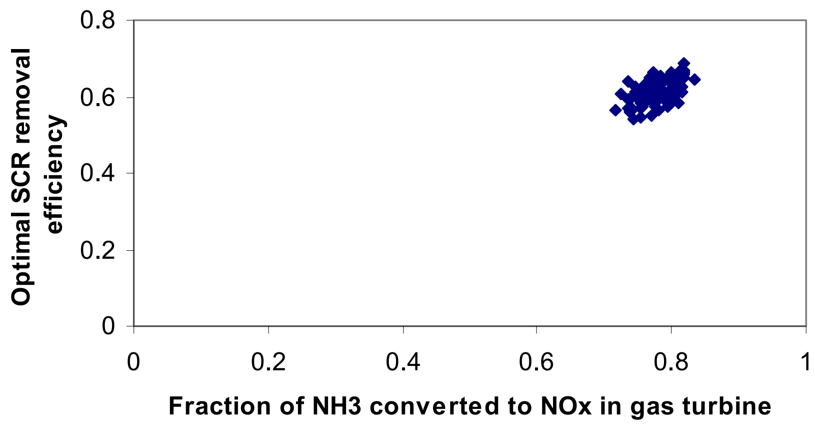


Figure 5-18. Dependence of Optimal SCR Removal Efficiency on the Fraction of NH3 Converted to NO_X in Gas Turbine

between the optimal SCR NO_X removal efficiency and XXCRN (Sample correlation coefficient is 0.91). Dependence of optimal SCR NO_X removal efficiency on XXNH3 is not as strong as on XXCRN. However, the correlation is still statistically significant on a 95% level of confidence (Sample correlation coefficient is 0.55).

To identify the key variables that contribute uncertainty in cost of electricity, correlation coefficient between optimal cost of electricity (which means that design variables

Table 5-9. Four Key Contributors to the Uncertainty in the Optimal Cost of Electricity

Variable Name	Correlation Coefficient with the Optimal Cost of Electricity *
Zinc ferrite absorption attrition rate (% loss per cycle)	0.875
Project contingency factor	0.377
Error term of HRSG direct cost of model ($Millions)	0.364
Unit cost of coal ($/lb)	0.321

*: All coefficients shown are statistically significant at a 95% level of confidence

are at optimal values) and random samples of each uncertain variable are calculated. Correlation coefficient provides an estimate of the linear dependence of a model output on a particular model input, and is a way for identifying key contributors to uncertainty (Cullen and Frey, 1999). Four statistically significant key contributors were identified and are given in Table 5-9 along with their correlations with the optimal cost of electricity. Zinc ferrite absorption attrition rate was found to be the key contributor to the uncertainty in the optimal cost of electricity. Thus, resolving uncertainty in zinc ferrite absorption attition rate is of significant importance to reducing uncertainty in the optimal cost of electricity.

Stochastic programming was conducted when NO_X emissions are constrained to less than or equal to 0.1 lb/10^6Btu and 0.3 lb/10^6Btu, respectively. The results are qualitatively similar to the case when NO_X emissions are constrained to less than or equal to 0.2 lb/10^6Btu. Average values and 95% range of both optimal cost of electricity and optimal design values are summarized in Table 5-10 for all three of these constraints. At optimal points for all the three constraints, RMOXG2C is at the lower bound, XSLCNV and CF are at the high bounds. This is consistent with sensitivity of cost of electricity to these variables as shown in Figure 5-2, 5-4 and 5-7. Variations in optimal values of RSTM2OX, XNH3S are due to that the cost of electricity is not sensitive to them as shown in Figure 5-3 and 5-6. Optimal values of REPHRS vary only by a very small percentage of its mean values. Variations of optimal

Table 5-10. Minimization of Cost of Electricity in Stochastic Programming when Considering Uncertainty in Model Inputs

	Level 1	Level 2	Level 3
Constraint on NO_X Emissions ($lb/10^6Btu$)	NO_X emissions ⩽0.3	NO_X emissions ⩽0.2	NO_X emissions ⩽0.1
Mean Value of the Optimal cost of electricity (mills/kWh)	51.46	51.61	51.86
95% range of optimal cost of electricity (mills/kWh)	48.07 ~ 60.15	48.25 ~ 60.30	48.48 ~ 60.54
Mean value of optimal RMOXG2C	0.45	0.45	0.45
95% range of optimal RMOXG2C	0.45 ~ 0.45	0.45 ~ 0.45	0.45 ~ 0.45
Mean value of optimal RSTM2OX	0.455	0.453	0.453
95% range of optimal RSTM2OX	0.454 ~ 0.455	0.450 ~ 0.455	0.450 ~ 0.455
Mean value of optimal XSLCNV	0.95	0.95	0.95
95% range of optimal XSLCNV	0.95 ~ 0.95	0.95 ~ 0.95	0.95 ~ 0.95
Mean value of optimal SCRAE	0.50	0.62	0.82
95% range of optimal SCRAE	0.50 ~ 0.50	0.56 ~ 0.67	0.79 ~ 0.84
Mean value of optimal XNH3S	5.2	8.8	9.5
95% range of optimal XNH3S	5.0 ~ 5.6	5.3 ~ 12.8	5.0 ~ 18.0
Mean value of optimal CF	0.9	0.9	0.9
95% range of optimal CF	0.9 ~ 0.9	0.9 ~ 0.9	0.9 ~ 0.9
Mean value of optimal REPHRS	25000	24678	24878
95% range of optimal REPHRS	25000 ~ 25000	23900 ~ 25000	24600 ~ 25000

values for SCRAE are due to uncertainty associated with mean value in XXNH3 and XXCRN as discussed in Section 5.1.2. When NO_X emissions is constrained to be not greater than 0.3 lb/106Btu, the optimal SCR removal efficiency stays at 0.50 without any change. This suggests that the lowest SCR removal efficiency of 0.50 can meet NO_X emissions constraint no matter changes in XXNH3 and XXCRN.

5.2.3 Comparison of Stochastic Optimization and Stochastic Programming Results

Comparison between the optimal expected value from stochastic optimization and average optimal value from stochastic programming enables one to evaluate the EVPI. Table 5-11 summarizes the EVPI for three levels (different NO_X emissions' constraint) that have been done, when uncertainty in model inputs is considered. In stochastic optimization, when the 90th percentile of NO_X emissions is constrained to be less than or equal to 0.2 lb/10^{6}Btu, the optimal expected cost of electricity is 51.65 mills/kWh. This value is 0.04 mills/kWh higher than the average optimal cost of electricity from stochastic programming in which NO_X emissions are constrained to be not greater than 0.2 lb/10^{6}Btu. If the loss function is the cost of electricity, then EVPI for this case is 0.04 mills/kWh, or 0.24 million dollars per year. We used 90th percentile of NO_X emissions as constraint in stochastic optimization; other statistics, such as expected value or 95th percentile are also applicable. It is up to decision makers as to how much reliability in NO_X emissions they need in stochastic optimization design. Figure 5-19 shows the NO_X emissions for each realization of uncertainty under the optimal designs of both stochastic optimization and stochastic programming. For each realization of uncertainty, the stochastic programming ensures that NO_X emissions are less than 0.2 lb/10^{6}Btu, while stochastic optimization ensures that 90% of NO_X emissions are less than 0.2 lb/10^{6}Btu, and there is violation for the rest 10%. The reason for the positive EVPI is

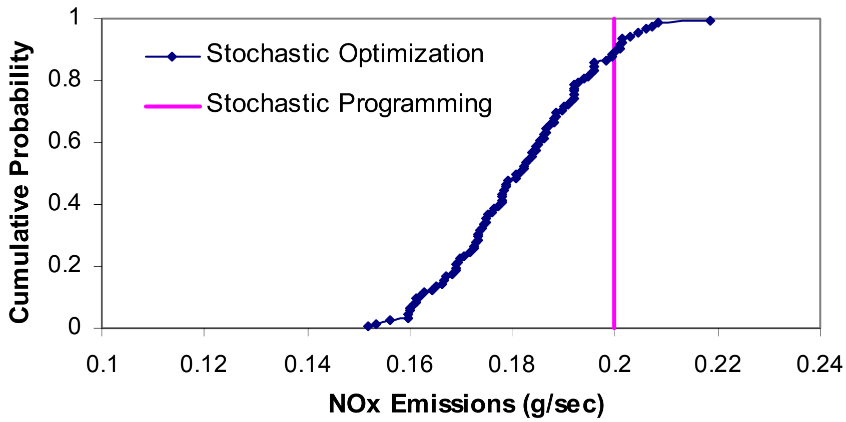


Figure 5-19. NO_X Emissions for Each Realization of Uncertainty under the Optimal Designs of both Stochastic Optimization and Stochastic Programming

that in stochastic optimization, the required SCR removal efficiency is 65%, which is 3% higher than average SCR removal efficiency in stochastic programming. As shown in Figure 5-5, higher SCR removal efficiency leads to higher cost of electricity. For the case in which NO_X emissions are constrained by 0.3 lb/10^6Btu, EVPI is 0, since there is no difference between the optimal SCR removal efficiency in stochastic optimization and average optimal SCR removal efficiency in stochastic programming. In the case 3, optimal expected cost of electricity was 51.88 mills/kWh from stochastic optimization when 90^{th} percentile of NO_X emissions is constrained to be not greater than 0.1 lb/10^6Btu. This value is 0.02 higher than the average optimal cost of electricity from stochastic programming in which NO_X emissions are constrained to be not greater than 0.1 lb/10^6Btu. EVPI is 0.02 mills/kWh in this case. This value is lower than that of Level 2, which is 0.04 mills/kWh. The reason is that in this case, the difference in SCR removal efficiency between stochastic optimization and stochastic programming is only 1%, while in the level 2, the difference in SCR removal efficiency between stochastic optimization and stochastic programming is 3%; meanwhile, cost of electricity is linearly correlated with SCR removal efficiency as shown in Figure 5-5.

Table 5-11. Comparison of Stochastic Optimization and Stochastic Programming Results when Uncertainty in Model Inputs is Considered

	Level 1	Level 2	Level 3
Stochastic Optimization Results			
NO_X emission constraint	Probability (NO_X emissions $\leq 0.3) \geq 0.90$	Probability (NO_X emissions $\leq 0.2) \geq 0.90$	Probability (NO_X emissions $\leq 0.1) \geq 0.90$
Minimum expected cost of electricity	51.46	51.65	51.88
SCR Removal Efficiency	0.50	0.65	0.83
Stochastic Programming Results			
NO_X emission constraint	NO_X emissions $\leqslant 0.3$	NO_X emissions $\leqslant 0.2$	NO_X emissions $\leqslant 0.1$
Mean value of cost of electricity	51.46	51.61	51.86
Mean value of SCR removal efficiency	0.50	0.62	0.82
Expected Value of Perfect Information			
Mills/kWh	0.00	0.04	0.02
10^6\$/Year	0.00	0.24	0.12

5.3 Optimization Considering both Variability and Uncertainty in Model Inputs

In the previous two sections, optimization of the IGCC system was conducted when only variability or only uncertainty in model inputs is considered. In this section, optimization is conducted for the same problem simultaneously considering both variability and uncertainty in model inputs.

As discussed in Chapter 3, 27 model inputs were identified with uncertainty. Probability distributions for these 27 variables are given in Table 3-3. For each variable with uncertainty, 100 random samples were generated from AuvTool. The other 26 model inputs were identified to have both variability and uncertainty. Probability distributions for these inputs are given in Table 3-5. For each variable with both variability and uncertainty, 100 samples for variability and 100 realizations for uncertainty were generated using AuvTool.

As discussed in Chapter 2, two methods are proposed for optimization considering both variability and uncertainty in model inputs. The first method, termed as a coupled stochastic optimization and programming technique, features stochastic optimization for each realization of variability (alternative frequency distribution in bootstrap simulation). The output of this method forms probability distributions for optimal results from stochastic optimization. The second method, termed as a two-dimensional stochastic programming method, involves deterministic optimization at each iteration of random samples for variability and uncertainty. The outputs from this method are two-dimensional distributions for optimal results from deterministic optimization.

5.3.1 Results from Coupled Stochastic Optimization and Programming Technique

One case study is done to demonstrate the coupled stochastic optimization and programming technique, In this case, for each realization of uncertainty, stochastic optimization is carried out in search of the optimal expected cost of electricity when the 90th percentile of NO_X emissions is constrained to be less than or equal to 0.2 lb/10^6Btu. Because there are 100 realizations for uncertain inputs, stochastic optimization is processed for 100 times. Each stochastic optimization is conducted considering variability in inputs. Figure 5-20 presents the cumulative probability distribution for the optimal expected cost of electricity from the coupled stochastic optimization and programming method. The average value of optimal expected cost of electricity is 51.73 mills/kWh, and 90% of the estimates of the optimal expected cost of electricity are less than 55 mills/kWh. Correlation coefficients between the optimal expected cost of electricity and random numbers for each uncertain variable were calculated to identify the key contributors to uncertainty in the optimal expected cost of electricity. Table 5-12 lists the four statistically significant key contributors

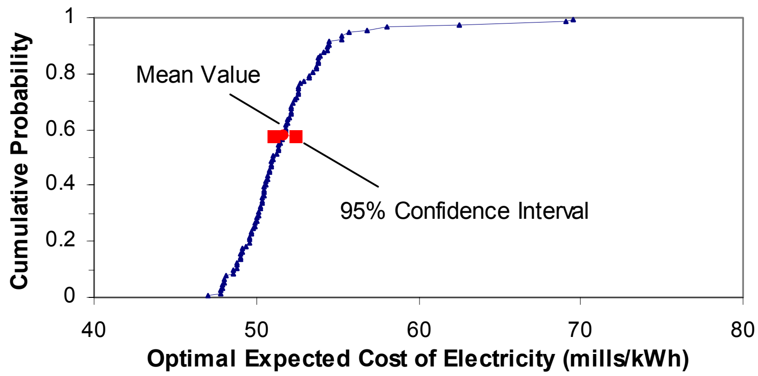


Figure 5-20. Cumulative Probability Distribution for Optimal Expected Cost of Electricity from the Coupled Stochastic Optimization and Programming Method when 90th Percentile of NO_X emissions ≤ 0.2 lb/10^6Btu

Table 5-12. Key Contributors to the Uncertainty in the Optimal Expected Cost of Electricity

Variable Name	Correlation Coefficient with the Optimal Cost of Electricity *
Zinc ferrite absorption attrition rate (% loss per cycle)	0.877
Project contingency factor	0.350
Error term of HRSG direct cost of model ($Millions)	0.341
Unit cost of coal ($/lb)	0.312

*: All coefficients are all statistically significant at a 95% level of confidence

along with the correlation coefficients. Among them, zinc ferrite absorbent attrition rate was found to be the key contributor. This is consistent with the conclusion in Section 5.2.2. Figure 5-21 shows the cumulative probability distribution for optimal SCR removal efficiency. The average optimal SCR removal efficiency is 0.70, with a 95% range from 0.65 to 0.74. Table 5-13 summarizes the average value and 95% range for other design variables. For the 100 realizations of stochastic optimization, optimal values for all other design variables vary very little except SCR removal efficiency.

The computational burden is heavy for the coupled stochastic optimization and programming technique. This particular case study took 4 hours and 30 minutes to complete on a Pentium 4, 2.4 GHz desktop computer.

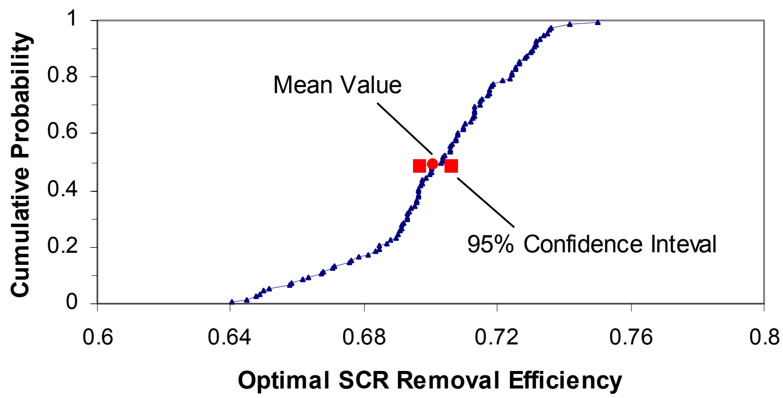


Figure 5-21. Cumulative Probability Distribution for the Optimal SCR Removal Efficiency from the Coupled Stochastic Optimization and Programming Method when the 90th Percentile of NO_X Emissions ≤ 0.2 lb/10^{6}Btu

Table 5-13. Summary of the Optimal Results from the Coupled Stochastic Optimization and Stochastic Programming when the 90th Percentile of NO_X Emissions ≤ 0.2 lb/10^{6}Btu

	Mean Value of Optimal Result	95% Range of the Optimal Values
Expect Cost of Electricity (mills/kWh)	51.73	48.05 ~ 60.37
RMOXG2C	0.45	0.45 ~ 0.45
RSTM2OX	0.455	0.455 ~ 0.455
XSLCNV	0.95	0.95 ~ 0.95
SCRAE	0.70	0.65 ~ 0.74
XNH3S (ppm)	5.0	5.0 ~ 5.2
CF	0.9	0.9 ~ 0.9
REPHRS	25000	24998 ~ 25000

5.3.2 Results from the Two-dimensional Stochastic Programming Technique

Two dimensional stochastic programming involves deterministic optimization for each combination of random numbers sampled for variability and uncertainty. One case study is developed. In this case, during each deterministic optimization, the objective is to minimize the cost of electricity, where NO_X emissions are constrained to be less than or equal to 0.2 lb/10^{6}Btu. Since there are 100 random samples for variability and 100 realizations for uncertainty, 100×100 deterministic optimizations were done.

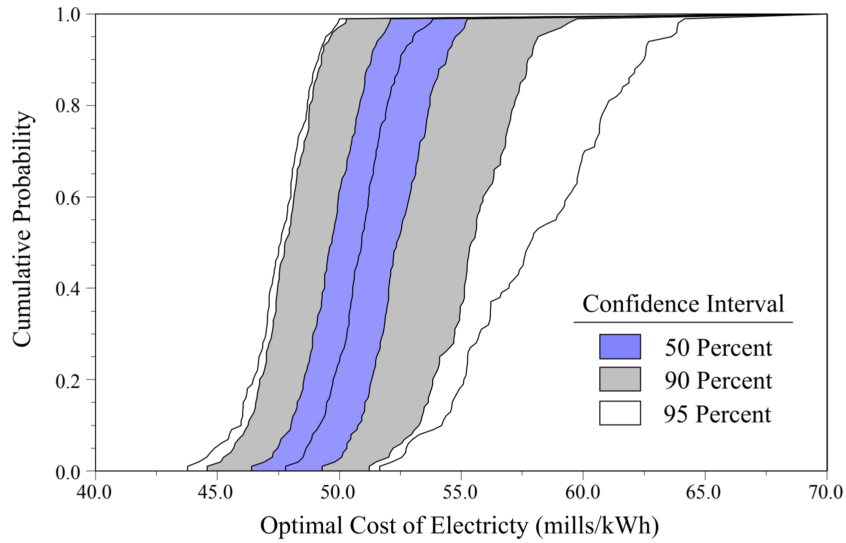


Figure 5-22. Two-dimensional Distributions for Minimum Cost of Electricity from the Two-dimensional Stochastic Programming Method when NO_X Emissions ≤ 0.2 lb/10^6Btu

Figure 5-22 shows the two dimensional probability distribution of the optimal cost of electricity for this case study. The average optimal cost of electricity is 51.62 mills/kWh with a 95% confidence interval on the mean from 47.67 mills/kWh to 60.35 mills/kWh. Sample correlation coefficients between the optimal cost of electricity and random numbers for variability and uncertainty were calculated to identify the key contributors to variability and uncertainty in the optimal cost of electricity. Table 5-14 summarizes the statistically significant key contributors to variability and uncertainty in the optimal cost of electricity, respectively. Zinc ferrite sorbent attrition rate (FATTZF) was found to be the most important contributor to the uncertainty in the optimal cost, while contingency in gas turbine (FPCG) was the most important contributor to the variability in the optimal cost.

Figure 5-23 shows the two dimensional probability distribution of optimal SCR removal efficiency. The average optimal SCR removal efficiency is 0.60, with a 95% confidence interval on the mean from 0.56 to 0.66. As the SCR removal efficiency is

Table 5-14. Key Contributors to the Variability and Uncertainty in the Optimal Cost of Electricity

Key Contributors to the Variability in the Optimal Cost of Electricity		Key Contributors to the Uncertainty in the Optimal Cost of Electricity	
Variable	Correlation Coefficient *	Variable	Correlation Coefficient *
Process contingency in gas turbine	0.487	Zinc ferrite absorption attrition rate	0.877
Process contingency in gasifier	0.398	Project contingency factor	0.349
Unit cost of zinc ferrite absorbent ($/lb)	0.365	Error term of HRSG direct cost of model	0.340
Maintenance factor for gas turbine	0.283	Unit cost of coal ($/lb)	0.312
Maintenance factor for gasifier	0.240		

*: All coefficients are statistically significant at a 95% level of confidence

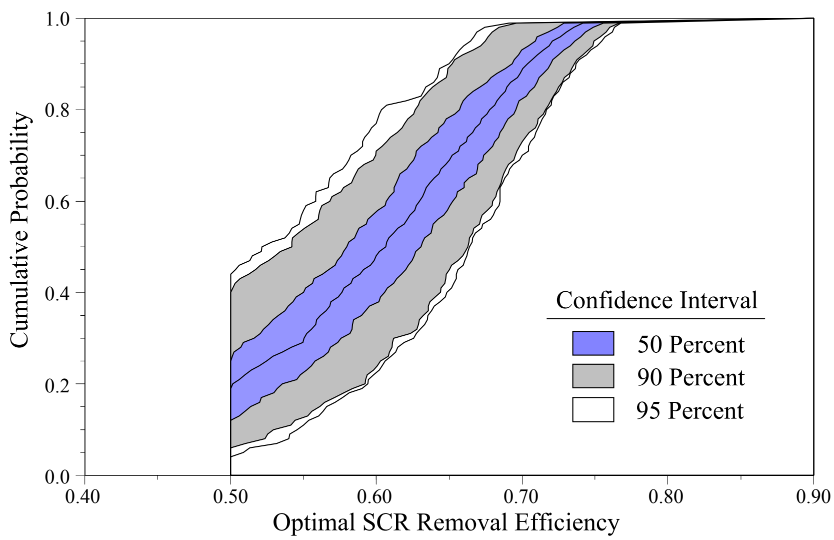


Figure 5-23. Two-dimensional Distributions for Optimal SCR Removal Efficiency from the Two-dimensional Stochastic Programming when NO_X Emissions ≤ 0.2 lb/10^6Btu

constrained to be not less than 0.50, the optimal SCR removal efficiency should be not less than 0.50 as reflected in the Figure 5-23.

The average value and the 95% confidence interval of the mean for optimal values of other design variables are summarized in Table 5-15. Optimal values for gasifier oxygen to

Table 5-15. Summary of Optimal Results from the Two-dimensional Stochastic Programming Method when NO_X Emissions $\leq 0.2 lb/10^6 Btu$

Variable	Average value	95% Range of the Mean
Cost of Electricity (mills/kWh)	51.62	47.67 ~ 60.35
Gasifier Oxygen to Carbon Ratio	0.450	0.450 ~ 0.450
Gasifier Steam to Carbon Ratio	0.453	0.452 ~ 0.454
Sulfur retained in the gasifier bottom ash	0.950	0.950 ~ 0.950
SCR NO_X Removal Efficiency	0.604	0.556 ~ 0.657
SCR ammonia slip (ppm)	8.1	6.8 ~ 9.4
Plant Capacity Factor	0.90	0.90 ~ 0.90
SCR Replacement Interval (hours)	24748	24534 ~ 24905

carbon ratio (RMOXG2C), sulfur retained in the gasifier bottom ash (XSLCNV) and capacity factor (CF) stay the same for all 10,000 deterministic optimizations. Optimal values for gasifier steam to carbon ratio (RSTM2OX) and SCR ammonia slip (XNH3S) vary. However, the cost of electricity is not sensitive to them (See Figure 5-3 and 5-6). Variation of SCR replacement interval is within 24,000 to 25,000 hours, in which range, cost of electricity is not sensitive (See Figure 5-8). SCR NO_X removal efficiency varies due to change in sample values during each deterministic optimization.

The computational burden associated with two-dimensional stochastic programming is very heavy. This case study costs approximately 20 hours to complete on a Pentium 4, 2.4 GHz desktop computer, which is about 4 fold more than the coupled stochastic optimization and programming technique. For comparison, computational time for stochastic optimization and stochastic programming are given in Table 5-16. Computational burden for stochastic optimization and stochastic programming when considering uncertainty is heavier than those when considering variability. This is due to the fact that both uncertainty in uncertain variables and uncertainty in the mean of the variables with variability and uncertainty were considered when doing optimization under uncertainty, while only variability in the variables

Table 5-16. A Summary of Computational Time for Each Technique

Technique	Average Computational Time (on a Pentium 4, 2.4 GHz desktop computer)
Stochastic Optimization Considering Variability	3 minutes
Stochastic Programming Considering Variability	10 minutes
Stochastic Optimization Considering Uncertainty	4 minutes
Stochastic Programming Considering Uncertainty	15 minutes
Coupled Stochastic Optimization and Programming Method	4 hours
Two-dimensional Stochastic Programming	20 hours

with variability and uncertainty are considered when doing optimization considering variability. More variables were sampled for cases considering uncertainty, which increases the computational time in data reading from the random data file.

5.3.3 Comparisons of Results from Coupled Stochastic Optimization and Programming Technique and from the Two-dimensional Stochastic Programming Method

As discussed in Section 5.1.3, comparison between stochastic optimization and stochastic programming enables one to explore the expected value of perfect information (EVPI).

When comparing the results from coupled stochastic optimization and programming method and those from the two-dimensional stochastic programming, a probability distribution for EVPI will be obtained. The effect of uncertainty on EVPI can be evaluated from the distribution. Each EVPI is calculated this way: as stochastic optimization was conducted for each realization of variability in which 90^{th} percentile of NO_X emissions is constrained to be less than or equal to 0.2 lb/10^6Btu, and stochastic programming was conducted for each realization of variability in which NO_X emissions are constrained to be less than or equal to 0.2 lb/10^6Btu; One EVPI was calculated for each realization of

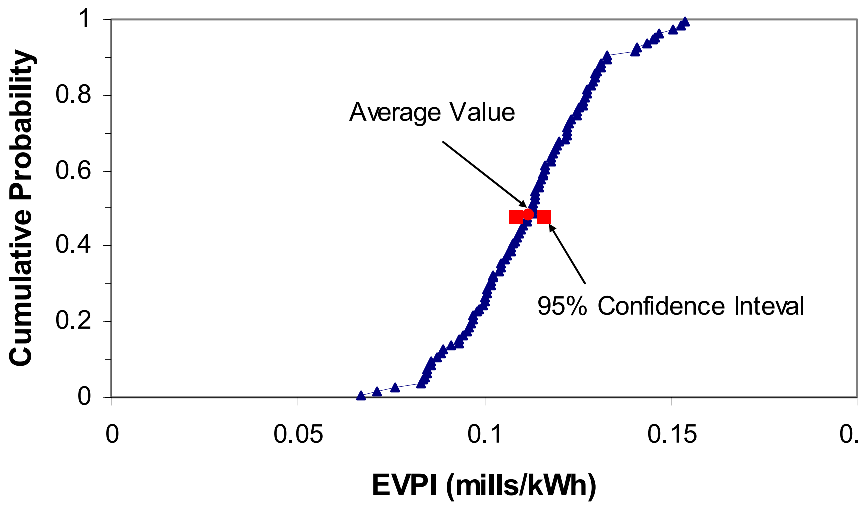


Figure 5-24. Cumulative Probability Distribution of Uncertainty in Expected Value of Perfect Information with respect to Variability

variability. Since 100 realizations of variability were sampled, 100 values of EVPI were obtained, which can be used to construct the probability distribution. Figure 5-24 is the probability distribution for EVPI. The average EVPI is 0.112 mills/kWh, which equals 0.7 million dollars per year. It is very close to the EVPI with the same constraints on NO_X emissions when considering only variability in model inputs, which is 0.10 mills/kWh. The 95% confidence interval on the mean is from 0.108 mills/kWh to 0.116 mills/kWh. 95% range of the EVPI extends from 0.08 mills/kWh to 0.15 mills/kWh. Based on the correlation coefficients between EVPI and samples for uncertain variables, no uncertain variables were found to be the key contributors to the uncertainty in EVPI at a 95% level of confidence.

Another attempt was to quantify the EVPI with regard to uncertainty in model inputs. Both the coupled stochastic optimization and programming method and the two-dimensional stochastic programming method were applied to multiple percentiles of variability.

In applying the coupled stochastic optimization and programming method, stochastic optimization was conducted for nine specified percentiles of variability, which were 1st, 5th,

Table 5-17. Summary of Optimal Results from the Coupled Stochastic Optimization and Programming Method which was applied to uncertainty with the 98th Percentile of NO_X Emissions ≤ 0.2 lb/10^6Btu

	Mean Value of Optimal Result	98% Probability Range of the Optimal Values
Expect Cost of Electricity (mills/kWh)	51.73	46.07 ~ 58.20
Gasifier Oxygen to Carbon Ratio	0.45	0.45 ~ 0.45
Gasifier Steam to Carbon Ratio	0.455	0.455 ~ 0.455
Sulfur retained in the Gasifier Bottom Ash	0.95	0.95 ~ 0.95
SCR NO_X Removal Efficiency	0.63	0.50 ~ 0.77
SCR Ammonia Slip (ppm)	5.0	5.0 ~ 5.0
Plant Capacity Factor	0.9	0.9 ~ 0.9
SCR Replacement Interval (hours)	25000	25000 ~ 25000

10th, 25th, 50th, 75th, 90th, 95th, and 99th percentile, respectively. During each stochastic optimization, the expected cost of electricity was minimized when the 90th percentile of NO_X emissions was constrained to be less than or equal to 0.2 lb/10^6Btu. The average optimal expected cost of electricity is 51.73 mills/kWh, and the 98% range of the optimal expected cost of electricity extends from 46.07 to 58.20 mills/kWh. The optimal design values are summarized in the Table 5-17.

In applying the two-dimensional stochastic programming method, stochastic programming was conducted for the same nine specified percentiles of variability, which were 1st, 5th, 10th, 25th, 75th, 90th, 95th, and 99th percentile, respectively. During each stochastic programming, the cost of electricity was minimized when the NO_X emissions were constrained to be less than or equal to 0.2 lb/10^6Btu. The average optimal cost of electricity is 51.71 mills/kWh. The optimal design values are summarized in the Table 5-18.

Comparing the optimal expected cost of electricity from each stochastic optimization process of the coupled stochastic optimization and programming method, and the expected optimal cost of electricity from each stochastic programming process of the two-dimensional

Table 5-18. Summary of Optimal Results from the Two-dimensional Stochastic Programming Method which was Applied to when NOX Emissions ≤ 0.2lb/106Btu

Variable	Average value	95 % Range of the Mean
Cost of Electricity (mills/kWh)	51.71	45.54 ~ 57.92
Gasifier Oxygen to Carbon Ratio	0.450	0.450 ~ 0.450
Gasifier Steam to Carbon Ratio	0.454	0.452 ~ 0.454
Sulfur retained in the gasifier bottom ash	0.950	0.950 ~ 0.950
SCR NO_X Removal Efficiency	0.62	0.50 ~ 0.75
SCR ammonia slip (ppm)	7.4	5.0 ~ 9.4
Plant Capacity Factor	0.90	0.90 ~ 0.90
SCR Replacement Interval (hours)	24856	24588 ~ 2500

stochastic programming method, EVPI with regard to uncertainty was evaluated. The average EVPI was 0.022 mills/kWh, or $133,000 per year. EVPI for each of the nine selected percentile of variability was given in Table 5-19. For the 1st, 5th, and 10th percentile of variability, there is no benefit of reducing uncertainty, while from the 25th percentile of variability, reducing uncertainty is of benefit. For the 1st, 5th, and 10th percentile of variability, the lowest SCR removal efficiency is the optimal value both for stochastic optimization and stochastic programming, there is no difference between the optimal SCR removal efficiency in stochastic optimization and the average optimal SCR removal efficiency in stochastic programming, which results no benefit of reducing uncertainty. Starting from 25th percentile, since the optimal SCR removal efficiency in stochastic optimization is greater than the average optimal SCR removal efficiency in stochastic programming, so EVPI is positive. Optimal SCR removal efficiency depends on the value of fraction of coal bound nitrogen converted NH_3 in the gasifier and the fraction of NH_3 converted to NO_X in the gas turbine. At low percentiles of variability, the values of these two variables are low, so lowest SCR removal efficiency can satisfy the constraint on NO_X emissions.

Table 5-19. Summary of EVPI with regard to Uncertainty for the Selected Nine Percentiles of Variability

Percentile of the Variability	Optimal Expected Cost of Electricity from Stochastic Optimization [a]	Average Optimal Cost of Electricity from Stochastic Programming [b]	EVPI (mills/kWh)	EVPI (10^6\$/year)
1st percentile	45.18	45.18	0	0
5th percentile	46.07	46.07	0	0
10th percentile	46.80	46.80	0	0
25th percentile	48.62	48.58	0.04	0.24
50th percentile	51.56	51.51	0.05	0.30
75th percentile	54.70	54.67	0.03	0.18
90th percentile	56.88	56.85	0.03	0.18
95th percentile	57.55	57.52	0.03	0.18
99th percentile	58.20	58.18	0.02	0.12

[a]: Stochastic optimization was conducted considering uncertainty in a certain percentile of variability; the expected cost of electricity was minimized when the 90th percentile of NO_X emissions was less than or equal to 0.2 lb/10^6Btu;

[b]: Stochastic programming was conducted considering uncertainty in a certain percentile of variability, cost of electricity was minimized when the NO_X emissions were less than or equal to 0.2 lb/10^6Btu.

5.4 Summary of Results

Optimization of NO_X emissions control in an IGCC system was conducted when variability and/or uncertainty in model inputs are considered. A series of case studies were done. This section summarizes the main results from these case studies.

Section 5.1 presented optimization results when only variability in model inputs is considered. During stochastic optimization, the expected cost of electricity was optimized when the 90th percentile of NO_X emissions was constrained; while during stochastic programming, for each realization of variability, the cost of electricity was optimized when NO_X emissions were constrained. Table 5-20 summarizes the comparisons between the optimal expected cost of electricity from stochastic optimization and the average optimal cost of electricity from stochastic programming when variability in model inputs is considered.

Table 5-20. Summary of Stochastic Optimization and Stochastic Programming Results when Variability in Model Inputs is Considered

	Level 1	Level 2	Level 3
Stochastic Optimization Results			
NO_X emission constraint	Probability (NO_X emissions $\leq 0.3) \geq 0.90$	Probability (NO_X emissions $\leq 0.2) \geq 0.90$	Probability (NO_X emissions $\leq 0.1) \geq 0.90$
Minimum expected cost of electricity	50.35	50.55	50.76
Stochastic Programming Results			
NO_X emission constraint	NO_X emissions $\leqslant 0.3$	NO_X emissions $\leqslant 0.2$	NO_X emissions $\leqslant 0.1$
Mean value of cost of electricity	50.35	50.45	50.71
Expected Value of Perfect Information (EVPI)			
Mills/kWh	0.00	0.15	0.05
10^6\$/Year	0.00	0.60	0.30

Section 5.2 presented optimization results when only uncertainty in model inputs is considered. During stochastic optimization, the expected cost of electricity was optimized when the 90th percentile of NO_X emissions was constrained; while during stochastic programming, for each realization of uncertainty, the cost of electricity was optimized when NO_X emissions were constrained. Table 5-21 summarizes the comparisons between the optimal expected cost of electricity from stochastic optimization and the average optimal cost of electricity from stochastic programming when uncertainty in model inputs is considered.

Section 5.3 presented optimization results when both variability and uncertainty in model inputs are considered. One case study was done with regard to variability using both the coupled stochastic optimization and programming method and the two-dimensional stochastic programming method. During the coupled stochastic optimization and programming method, the 90th percentile of NO_X emissions was constrained to be less than or equal to 0.2 lb/10^6Btu for each stochastic optimization process. During the two-dimensional stochastic programming process, NO_X emissions were constrained to be less

Table 5-21. Summary of Stochastic Optimization and Stochastic Programming Results when Uncertainty in Model Inputs is Considered

	Level 1	Level 2	Level 3
Stochastic Optimization Results			
NO_X emission constraint	Probability (NO_X emissions ≤ 0.3) ≥ 0.90	Probability (NO_X emissions ≤ 0.2) ≥ 0.90	Probability (NO_X emissions ≤ 0.1) ≥ 0.90
Minimum expected cost of electricity	51.46	51.65	51.88
Stochastic Programming Results			
NO_X emission constraint	NO_X emissions $\leqslant 0.3$	NO_X emissions $\leqslant 0.2$	NO_X emissions $\leqslant 0.1$
Mean value of cost of electricity	51.46	51.61	51.86
Expected Value of Perfect Information (EVPI)			
Mills/kWh	0.00	0.04	0.02
10^6\$/Year	0.00	0.24	0.12

than or equal to 0.2 lb/10^6 Btu for each deterministic optimization process. A probability distribution for EVPI was constructed through comparing the results from the two methods. Average value of EVPI was 0.112 mills/kWh with a 95% confidence interval between 0.108 and 0.116 mills/kWh. Another case study was done with regard to uncertainty in selected 9 percentiles of variability using both the coupled stochastic optimization and programming method and the two-dimensional stochastic programming method. Similarly, during the coupled stochastic optimization and programming method, the 90th percentile of NO_X emissions was constrained to be less than or equal to 0.2 lb/10^6Btu for each stochastic optimization process. During the two-dimensional stochastic programming process, NO_X emissions were constrained to be less than or equal to 0.2 lb/10^6 Btu for each stochastic programming process. Average EVPI was found to be 0.022 mills/kWh, or \$133,000 per year.

6.0 CONCLUSIONS AND RECOMMENDATIONS

This study combines optimization techniques with probabilistic analysis for robust design of process technologies. Stochastic optimization and stochastic programming techniques are available for optimization of process models when uncertainty in model inputs is considered. A coupled stochastic optimization and programming technique, and two-dimensional stochastic programming methods are proposed in this study for optimization of process models when both variability and uncertainty in model inputs are considered. These techniques are then applied to a case study of NO_X emissions control in an IGCC system.

The main work and major findings of the study are as follows:

1. Genetic Algorithm performs well for optimization of process models based on comparisons with traditional mathematical programming methods and sensitivity analysis with regard to the dependence of the cost of electricity on the design variables;
2. To minimize the cost of electricity of the IGCC system, gasifier oxygen to carbon ratio should be kept at 0.45; sulfur retained in the gasifier bottom ash should be kept at 0.95; SCR catalyst layer replacement interval should be kept at 25,000 hours; and capacity factor should be at 0.90. Controls of the gasifier steam to carbon ratio and SCR ammonia slip do not have a substantial effect on the cost of electricity with the range of values considered, although high gasifier steam-to-carbon ratio and low SCR ammonia slip can slightly decrease the cost of electricity (but by no more than 0.01 mills/kWh). The specification of SCR removal efficiency depends on the NO_X

emissions constraints. High SCR removal efficiency results in an increase with the cost of electricity, but lowers NO_X emissions;

3. Stochastic optimization and stochastic programming are applied to the IGCC model when only variability in model inputs is considered. Stochastic programming results indicate that the variability in model inputs can have substantial effect on the optimal cost of electricity. Expected Value of Perfect Information (EVPI) is calculated as the difference between optimal expected cost of electricity from stochastic optimization and expected optimal cost of electricity from stochastic programming. EVPI is about 0.6 million dollars on a yearly basis when NO_X emissions are constrained to be not greater than 0.2 lb/10^6Btu in stochastic programming, and 90th percentile of NO_X emissions is constrained to be less than or equal to 0.2 lb/10^6Btu in stochastic optimization. This is the benefit if the decision variables can be adjusted according to site specific or time specific realizations of variability.
4. Stochastic optimization and stochastic programming are also applied to the IGCC system when only uncertainty in model inputs is considered. Stochastic programming results indicate that uncertainty in model inputs can significantly increase the optimal cost of electricity. The most influential factor is the uncertainty associated with zinc ferrite sorbent attrition rate. Resolving uncertainty in zinc ferrite sorbent attrition rate is of highest priority;
5. The coupled stochastic optimization and programming technique, and two-dimensional stochastic programming method were applied to the IGCC model when both variability and uncertainty in model inputs are considered. From the two-dimensional stochastic programming method, key contributor to the variability in the

optimal cost of electricity was found to be process contingency factor in the gas turbine, while zinc ferrite absorbent attrition rate was the key contributor to uncertainty in the optimal cost of electricity. Computational burden with both these two methods are heavy. Coupled stochastic optimization and programming method took more than 4 hours to complete on a Pentium 4, 2.4 GHz desktop computer. Two-dimensional stochastic programming cost approximately 20 hours to complete on the same computer.

6. The combination of probabilistic analysis, optimization, and sensitivity analysis demonstrated in this study provides a powerful and rigorous tool for design of process technologies. Key contributors to the variability and uncertainty in the final optimal results were identified. These should be addressed by targeted research and development efforts.

Recommendations for future studies are given as follows:

1. This study is focused on optimization of cost of electricity for the IGCC system when NO_X emissions are constrained. Future study should also include SO_2 emissions as a constraint;
2. The IGCC system studied here features a KRW gasifier based system with hot gas cleanup. There are other designs of IGCC systems, based on Texaco, Shell, Lurgi, or Dow gasifier technologies (Frey and Rubin, 1990). The optimization under variability and/or uncertainty techniques used in this study can be applied to these IGCC systems;

3. Future study can consider a real-time online optimization problem. For the variables with variability, whether their values can be measured at real time or not should be examined. Meanwhile, adaptation of the design variables to the variables with variability or with uncertainty is easy or not should be addressed. Real time online optimization problem will be more complex but more interesting. Perhaps, a more comprehensive process model will be required.
4. In the current study, random numbers are generated off-line from AuvTool. A possible improvement to the software is to incorporate the random number generation capability into the existing framework under Excel, so that random numbers can be generated online.

7.0 REFERENCE

Bak, J., K. Tybirk (1998), "The EU Acidification Strategy: Sensitivity of calculated emission ceilings for nitrogen and sulphur for Denmark," *Environmental Pollution*, 102 (S1): 625-633

Bharvirkar, R., H.C. Frey (1998), *Development of Simplified Performance and Cost Models of Integrated Gasification Combined Cycle Systems*, Prepared by North Carolina State University for Center for Energy and Environmental Studies, Carnegie Mellon University, Pittsburg, PA.

Bjorge, R., *et al*. (1996), "IGCC Technology for the 21st Century," Session Number 5, *Proceedings, 1996 Gasification Technologies Conference*, Electric Power Research Institute, Palo Alto, CA.

Burn, D., J. S. Yulianti (2001), "Waste-Load Allocation using Genetic Algorithms," *Journal of Water Resources Planning and Management*, 127 (2): 121-129.

Chemical Week Publish, L.L.C. (2002), "Economic Indicators," *Chemical Engineering*, 109(3): 96.

Cocks, A.T., I.R. Rodgers, R.A. Skeffington, A.H. Webb (1998), "The limitations of integrated assessment modeling in developing air pollution control policies," *Environmental Pollution* 102 (S1), 635-639.

Cullen, A.C., H.C. Frey (1999), *Use of Probabilistic Techniques in Exposure Assessment: A Handbook for Dealing with Variability and Uncertainty in Models and Inputs*, Plenum Press: New York.

Dakins, M.E., T. E. John, S. J. Mitchell (1994), "Risk-based Environmental Remediation: Decision Framework and Role of Uncertainty," *Environmental Toxicology and Chemistry*, 13 (12): 1907-1915.

Dakins, M.E. (1999), "The Value of the Value of Information," *Hum. Ecol. Risk Assess.* 5(2), 281-289.

Dantus, M.M., K. A. High (1999), "Evaluation of Waste Minimization Alternatives under Uncertainty: a Multi-objective Optimization Approach," *Computers and Chemical Engineering*, 23(10): 1493-1508.

Diwekar, U.M., H.C. Frey, E.S. Rubin (1992), "Synthesizing Optimal Flow Sheets: Applications to IGCC System Environmental Control," *Ind. Eng. Chem. Res.* 31(8): 1927-1936.

Diwekar, U.M., E.D. Rubin, H.C. Frey (1997), "Optimal Design of Advanced Power Systems under Uncertainty," *Energy Conversion and Management*, 38(15-17):1725-1735.

Draper, D., J.S. Hodges, E.E. Leamer, C.N. Morris, D.B. Rubin (1987), *A Research Agenda for Assessment and Propagation of Model Uncertainty*, Report N-2683-RC, Rand Corporation, Santa Monica, California.

Efron, B., R. J. Tibshirani (1993), *An Introduction to the Bootstrap*, Chapman and Hall: New York, 1993.

EPA (1997), "Proposed Revision of Standards of Performance for Nitrogen Oxide Emissions from New Fossil-Fuel Fired Steam Generating Units; Proposed Revisions to Reporting Requirements for Standards of Performance for New Fossil-Fuel Steam Generating Units; Proposed Rule", *Federal Register*, 62(131): 36,948-36,963 (Preamble to proposed regulation 40 Code of Federal Regulations Part 60).

EPRI (1988), *Cool Water Coal Gasification Program: Fifth Annual Progress Report*, AP-4832, Electric Power Research Institute, Palo Alto, CA.

Fournier, R., M.A. Latifi, G. Valentin (1999), "Methodology of Dynamic Optimization and Optimal Control of Batch Electrochemical Reactors," *Chemical Engineering Science* 54(14): 2707-2714.

Frey, H.C. and E.S. Rubin (1990), *Stochastic Modeling of Coal Gasification Combined Cycle Systems: Cost Models of Selected Integrated Gasification Combined Cycle (IGCC) Systems*, Topical Report, DOE/MC/24248-2901, NTIS DE90015345, Prepared by Carnegie-Mellon University for the U.S. Department of Energy, Morgantown, West Virginia.

Frey, H.C., E.S. Rubin (1991a), "Probabilistic Evaluation of Advanced SO_2/NO_X Control Technology," *J. Air. Waste Manage. Assoc.*, 41(12):1585-1593.

Frey, H.C., E.S. Rubin (1991b), *Development and Application of a Probabilistic Evaluation Method for Advanced Process Technologies*, Final Report, DOE/MC/24248-3015, NTIS DE91002095, Prepared by Carnegie-Mellon University for the U.S. Department of Energy, Morgantown, West Virginia.

Frey, H.C. (1992), *Quantitative Analysis of Uncertainty and Variability in Environmental Policy Making*, Directorate for Science and Policy Programs, American Association for the Advancement of Science, Washington, DC, 1992.

Frey, H.C., E.S. Rubin (1992a), "Integration of Coal Utilization and Environmental Control in Integrated Gasification Combined Cycle Systems," *Environmental Science Technology*, 26 (10): 1982-1990.

Frey, H.C., E.S. Rubin (1992b), "Evaluate Uncertainties in Advanced Process Technologies," *Chemical Engineering Progress*, 87(6): 63-70.

Frey, H.C., E.D. Rubin, U.M. Diwekar (1994), “Modeling Uncertainties in Advanced Technologies: Application to a Coal Gasification System with Hot-gas Cleanup,” *Energy*, 19 (4): 449-463.

Frey, H.C. (1994), *Development and Applications of Performance and Cost Models for Gas Turbine-Based Selective Catalytic Reduction NO_X Control*, Task 1Topical Report, Volume 1, DE-AC21-92MC29094, Prepared by North Carolina State University for Carnegie Mellon University and U.S. Department of Energy, Morgantown, WV.

Frey, H.C., D. Rhodes (1996), “Characterizing, Simulating and Analyzing Variability and Uncertainty: an Illustration of Methods using an Air Toxics Emissions Example,” *Human and Ecological Risk Assessment*, 2(4): 762-797.

Frey, H.C. (1997), “Variability and Uncertainty in Highway Vehicle Emission Factors,” *in Emission Inventory: Planning for the Future* (held October 28-30 in Research Triangle Park, NC), *Air and Waste Management Association*, Pittsburgh, Pennsylvania, pp. 208-219

Frey, H.C., D. Rhodes (1998), “Characterization and Simulation of Uncertain Frequency Distributions: Effects of Distribution Choice, Variability, Uncertainty, and Parameter Dependence,” *Human and Ecological Risk Assessment*, 4(2): 423-468.

Frey, H.C., and S. Bammi (2002), “Quantification of Variability and Uncertainty in Lawn and Garden Equipment NO_X and Total Hydrocarbon Emission Factors,” *Journal of the Air & Waste Management Association*, 52(4): 435-448.

Frey, H.C., and J. Zheng (2002), “Probabilistic Analysis of Driving Cycle-Based Highway Vehicle Emission Factors,” *Environmental Science and Technology*, 36(23): 5184-5191.

Frey, H.C, J. Zheng, Y. Zhao, S. Li., Y. Zhu (2002), *Technical Documentation of AuvTool Software Tool for Analysis of Variability and Uncertainty*, Prepared by North Carolina State University for Office of Research and Development, EPA, Research Triangle Park, NC.

Frey, H.C., K. Zhang (2003), “Probabilistic Analysis of Variability and Uncertainty in Process Technologies: A Case Study on KRW gasifier based IGCC System,” In Preparation.

Gen, M., R. Cheng (1997), *Genetic Algorithm and Engineering Design*, Wiley: New York.

George, T., P. Javier, L. Lin, T. Tawfik, R. Sears, D. Gallaspy (1992), “Cost-of-Electricity Minimization for an IGCC Power Plants,” Paper Number. 92-JPGC-Pwr-41, *International Power Generation Conference*, ASME, NY, Oct 18-22, 1992.

Gjerde, J., S. Grepperud, R. Kvernodokk (1999), “Optimal climate policy under the possibility of a catastrophe,” *Resource and Energy Economics*, 21(3-4): 289-317.

Holland, J.H. (1975), *Adaptation in Natural and Artificial Systems*, University of Michigan Press: Ann Arbor, MI.

Hou, K.F., Y. Li, J. Shen, S. Hu (2002), "Delayed Sampling Approach to Stochastic Programming in Chemical Processes," *Computers and Chemical Engineering*, 24(2-7): 619-624.

Ierapetritou, M. G., E. N. Pistikopoulos, C. A. Floudas (1996), "Operational Planning under Uncertainty," *Computers Chem. Engng.*, 20 (12): 1499-1516.

Nordhaus, W.D., D. Popp (1997), "What is the Value of Scientific Knowledge? An Application to Global Warming using the PRICE Model," *The Energy Journal*, 18 (1): 1-46.

Kim, K. J., U. M. Diwekar (2002a), "Efficient Combinatorial Optimization under Uncertainty. 1. Algorithmic Development," *Ind. Eng. Chem. Res.*, 41(5):1276-1284.

Kim, K. J., U. M. Diwekar (2002b), "Efficient Combinatorial Optimization under Uncertainty. 2. Application to Stochastic Solvent Selection," *Ind. Eng. Chem. Res.*, 41(5): 1285-1296.

L'Ecuyer, P. (1996), "Combined Multiple Recursive Random Number Generators," *Operations Research*, 44(5): 816-822.

Loughlin, D.H., S. Ranjithan, J.W. Baugh, E.D. Brill (2000), "Application of Genetic Algorithms for the Design of Ozone Control Strategies," *Journal of the Air and Waste Management Association*, 50(6): 1050-1063.

Morgan, M.G., M. Henrion (1990), *Uncertainty: A Guide to Dealing with Uncertainty in Quantitative Risk and Policy Analysis*, Cambridge University Press: New York.

NRC (1994), *Science and Judgment in Risk Assessment*, National Academy Press, Washington, D.C.

Palisade Corp. (1998), *Evolver: The Genetic Algorithm Super Solver for Microsoft Excel*, Palisade Corporation, Newfield, NY.

Pham, D.T., D. Karaboga (1998), *Intelligent Optimization Techniques*, Springer: London.

Pinto, J. C. (1998), "On the Costs of Parameter Uncertainties: Effect of Parameter Uncertainties during Optimization and Design of Experiments," *Chemical Engineering Science*, 53 (11), 2029-2040.

Rooney, W.C., L.T. Biegler (2003), "Optimal Process Design with Model Parameter Uncertainty and Process Variability," *AIChE Journal*, 49(2): 438-449.

Rubin, E.S., J.R. Kalagnanam, H.C. Frey, M.B. Berkenpas (1997), "Integrated Environmental Control Modeling of Coal-Fired Power Systems," *J. Air & Waste Manage. Assoc.*, 47(11): 1180-1188.

Shih, J., H.C. Frey (1995), "Theory and Methodology: Coal Blending Optimization under Uncertainty," *European Journal of Operational Research*, 83(3): 452-465.

U.S Department of Energy (2000), *Vision 21 Program Plan — Clean Energy Plants for the 21st Century*, Federal Energy Technology Center, Office of Fossil Energy, U.S. Department of Energy.

Wang, C., H. Quan, X. Xu (1996), "Optimal Design of Multi-product Batch Chemical Process Using Genetic Algorithms," *Ind. Eng. Chem. Res.* 35(10): 3560-3566.

Wardlaw, R., M. Sharif (1999), "Evaluation of Genetic Algorithms for Optimal Reservoir System Operation," *Journal of Water Resources Planning and Management*, 125 (1): 25-33.

Watanabe, T., H. Ellis (1993), "Stochastic Programming Models for Air Quality Management," *Computers & Operations Research*, 20(6): 651-663.

Tayal, M., Y. Fu, U.M. Diwekar (1999), "Optimal Design of Heat Exchangers: A Genetic Algorithm Framework," *Ind. Eng. Chem. Res.* ,38(2): 456-467.

Zheng, J., H.C. Frey (2002), "Development of a Software Module for Statistical Analysis of Variability and Uncertainty," paper # 12458, *Proceedings, Annual Meeting of the Air & Waste Management Association*, Pittsburgh, PA.

Zheng, J. (2002), *Quantification of Variability and Uncertainty in Emission Estimation: General Methodology and Software Implementation*, Ph.D. Dissertation, Department of Civil Engineering of North Carolina State University, Raleigh, NC.

Zheng, J., H.C. Frey, Y. Zhao, S. Li, Y. Zhu (2002), *Technical Documentation of AuvTool Software Tool for Analysis of Variability and Uncertainty*, Prepared by North Carolina State University for Office of Research and Development, US EPA, Research Triangle Park, NC.

Appendix A. INPUT AND OUTPUT FILES FOR PROCESS MODEL

Table A-1. Descriptions of Variables in the Input Files

Variable	Description
Configuration	Configuration of the process, which specify the choice of gas turbine and inclusion or exclusion of SCR
CARCNV	Gasifier Carbon Conversion
XCRCNV	Carbon Converted in Sulfation Unit
RMOXG2C	Gasifier Oxygen to Carbon Ratio
RSTM2OX	Gasifier Steam to Carbon Ratio
XXCRN	Fraction of Coal bound Nitrogen converted to NH_3
XXNH3	Fraction of NH_3 converted to NO_X in Gas Turbine
XSLCNV	Sulfur retained in Gasifier Bottom Ash
SCRAE	SCR NO_X removal Efficiency
XNH3S	SCR NH_3 Slip
A2	Parameter A2 used in equation (3-1) for determining RCAS from XSLCNV
B2	Parameter B2 used in equation (3-1) for determining RCAS from XSLCNV
FBM	Fraction of byproduct sales to marketing costs
FEHO	Factor of Engineering and home office fee
FGF	General facilities cost, fraction of other directs
FICC	Indirect Construction cost factor
FPJ	Project contingency factor
ALABOR	Average labor rate, including burdens ($/hour)
FPCCH	Process contingency of coal handling
FPCL	Process contingency of limestone handling
FPCOF	Process contingency of oxidant feed
FPCG	Process contingency of gasification
FPCS	Process contingency of sulfation
FPCZF	Process contingency of zinc ferrite
FPCBF	Process contingency of boiler feed water
FPCGT	Process contingency of gas turbine
FPCHR	Process contingency of heat recovery steam generator
FPCCR	Process contingency of selective catalytic reduction
FPCST	Process contingency steam turbine
FPCGF	Process contingency of general facilities
FMCCH	Maintenance cost factor of coal handling
FMCL	Maintenance cost factor of limestone handling
FMCOF	Maintenance cost factor of oxidant feed
FMCG	Maintenance cost factor of gasification
FMCS	Maintenance cost factor of sulfation

Table A-1 (Continued)

FMCZF	Maintenance cost factor of zinc ferrite
FMCBF	Maintenance cost factor of boiler feed water
FMCGT	Maintenance cost factor of gas turbine
FMCHR	Maintenance cost factor of heat recovery steam generator
FMCCR	Maintenance cost factor of selective catalytic reduction
FMCST	Maintenance cost factor of steam turbine
FMCGF	Maintenance cost factor of general facilities
BCCOAL	Unit cost of coal ($/MMBtu)
BCSAI	Unit cost of sulfuric acid ($/ton)
BCNAOH	Unit cost of NaOH ($/ton)
BCNA2H	Unit cost of Na2HPO4 ($/lb)
BCHYDR	Unit cost of Hydrazine ($/lb)
BCMORP	Unit cost of Morpholine ($/lb)
BCLIME	Unit cost of Lime ($/ton)
BCSODA	Unit cost of Soda Ash ($/ton)
BCCORI	Unit cost of Corrosion Inh. ($/lb)
BCSURF	Unit cost of Surfactant ($/lb)
BCCHLR	Unit cost of Chlorine ($/ton)
BCBIOC	Unit cost of Biocide ($/lb)
BCSCRC	Unit cost of SCR catalyst ($/ft^3)
BCNH3	Unit cost of Ammonia ($/ton)
BCZFSO	Unit cost of Zinc Ferrite Sorb ($/lb)
BCPLTA	Unit cost of Plant Air Ads ($/lb)
BCFLRL	Unit cost of LPG Flare ($/bbl)
BCWWCH	Unit cost of Waste Water ($/gpm ww)
BCFUEL	Unit cost of Fuel Oil ($/bbl)
BCRAWW	Unit cost of Raw Water ($/Kgal)
BCLMST	Unit cost of Limestone ($/ton)
BCASHD	Unit cost of Ash Disposal ($/ton)
SLZF	Zinc Ferrite sorbent sulfur loading, wt-% sulfur in sorbent
FATTZF	Zinc Ferrite sorbent attrition rate, wt-% sorbent loss per cycle
ERRHR	Error Term of HRSG direct cost model, $Million
ERRCR	Error Term of SCR direct cost model, $Million
ERRST	Error Term of Steam Turbine, $ Million

Example of an input file for the IGCC model

```
"Variables related to the Configuration"
2                    ! Configuration
.98                  ! CARCNV
.95                  ! XCRCNV
.47                  ! RMOXG2C
.455                 ! RSTM2OX
.1                   ! XXCRN
.9                   ! XXNH3
.80                  ! XSLCNV
.90                  ! SCRAE
20                   ! XNH3S
"Value of A2 and B2"
.233                 ! A2
.15                  ! B2
"Cost Model Parameters"
.65                 ! CF
.1                  ! FBM
.1                  ! FEHO
.2                  ! FGF
.2                  ! FICC
.175                ! FPJ
19.7                ! ALABOR
"Process Contingency"
.05                 ! FPCCH
.05                 ! FPCL
.1                  ! FPCOF
.2                  ! FPCG
.4                  ! FPCS
.4                  ! FPCZF
0                   ! FPCBF
.25                 ! FPCGT
.025                ! FPCHR
.1                  ! FPCCR
.025                ! FPCST
.05                 ! FPCGF
"Maintenance Cost Factors"
.03                 ! FMCCH
.03                 ! FMCL
.02                 ! FMCOF
.045                ! FMCG
.04                 ! FMCS
.03                 ! FMCZF
.015                ! FMCBF
.02                 ! FMCGT
```

(Continued from Page 92)

```
.015                    ! FMCHR
.02                     ! FMCCR
.015                    ! FMCST
.015                    ! FMCGF
"Variable Operating Costs"
1.61                    ! BCCOAL
110.0                   ! BCSAI
220.0                   ! BCNAOH
.7                      ! BCNA2H
3.2                     ! BCHYDY
1.3                     ! BCMORP
80.0                    ! BCLIME
160.0                   ! BCSODA
1.9                     ! BCCORI
1.25                    ! BCSURF
250.0                   ! BCCHLR
3.6                     ! BCBIOC
250.0                   ! BCSCRC
150.0                   ! BCNH3
3.0                     ! BCZFSO
2.8                     ! BCPLTA
11.7                    ! BCFLRL
840.0                   ! BCWWCH
42.0                    ! BCFUEL
.73                     ! BCRAWW
18.0                    ! BCLMST
10.0                    ! BCASHD
"Other Variables"
11390.0                 !  REPHRS
0.0                     !  ERRHR
0.17                    !  SLZF
0.8                     !  FATTZF
0.0                     !  ERRCR
0.0                     !  ERRST
```

Table A-2. Descriptions of Variables in the Output File

Variable	Description
WGTE	Gas Turbine Output (MWe)
WSTE	Steam Turbine Output (MWe)
WAUXE	Total Auxiliary Loads (MWe)
WNENE	Net Electricity (MWe)
DPERKW	Capital Cost ($/KW)
FOCN	Fixed Operating Cost ($/(KW-yr))
VOCINC	Incremental Variable Costs (mills/KWh)
BYPN	Byproduct Credit (mills/KWh)
FUELN	Fuel Cost (mills/KWh)
VOCN	Variable Operating Cost (mills/KWh)
CELEC	Cost of Electricity (mills/KWh)
HEATRATE	Heat Rate
EFFICNCY	Efficiency
MCOALIN	Coal Input (lb/KWh)
MH2OIN	Water Input (lb/KWh)
MLMSTIN	Limestone Input (lb/KWh
MASHOUT	Ash Outputs (lb/KWh)
MH2OOU	Water Outputs (lb/KWh)
ECO2	CO_2 Outputs (lb/KWh)
ESO2	SO_2 Outputs (lb/10^6Btu)
ENOX	NO_X Outputs (lb/10^6Btu)

Example of an output file for the IGCC model

Gas Turbine Output (MWe)
561.38
Steam Turbine Output (MWe)
311.31
Total Auxiliary Loads (MWe)
61.32
Net Electricity (MWe)
811.38
Capital Cost ($/KW)
425.51
Fixed Operating Cost ($/(KW-yr))
48.64
Incremental Variable Costs (mills/KWh)
4.25
Byproduct Credit (mills/KWh)
0.00
Fuel Cost (mills/KWh)
15.29
Variable Operating Cost (mills/KWh)
19.53
Cost of Electricity (mills/KWh)
53.96
Heat Rate
8364.80
Efficiency
0.40826
Coal Input (lb/KWh)
0.7436
Water Input (lb/KWh)
0.7984
Limestone Input (lb/KWh
0.2230
Ash Outputs (lb/KWh)
0.2120
Water Outputs (lb/KWh)
0.0488
CO2 Outputs (lb/KWh)
1.7157
SO2 Outputs (lb/MMBtu)
0.0131
NOX Outputs (lb/MMBtu)
0.0596

APPENDIX B. OPTIMIZATION UNDER VARIABILITY AND UNCERTAINTY FOR CONFIGURATION 2 IN THE IGCC MODEL

This appendix summarizes the results of optimization under variability and uncertainty for Configuration 2 in the simplified performance and cost model of IGCC systems. It includes results from

1. Stochastic optimization and stochastic programming when only considering variability in model inputs;
2. Stochastic optimization and stochastic programming when only considering uncertainty in model inputs;
3. Coupled stochastic optimization and programming, two-way stochastic programming when considering both variability and uncertainty in model inputs.

Optimization when Considering Variability in Model Inputs

Table B-1. Formulation of the Optimization Problem when Variability in Model Inputs is Considered

Configuration of the IGCC system:	Configuration 2: Gas Turbine with pressure ratio of 15.0 and turbine inlet temperature at 2350K, with Selective Catalytic Reduction (SCR)
Objective:	Minimization of Cost of electricity (mills/kWh) (For stochastic optimization, objective is minimization of expected value of cost of electricity; for stochastic programming, objective is minimization of cost of electricity at each sampling iteration)
Design variables:	1.Gasifier Oxygen to Carbon Ratio (RMOXG2C) 2.Gasifier Steam to Carbon Ratio (RSTM2OX) 3.Sulfer retained in the gasifier bottom ash (XSLCNV) 4.SCR NO_X Removal Efficiency (SCRAE) 5.SCR ammonia slip (XNH3S) 6.Plant Capacity Factor (CF) 7.SCR Replacement Interval (REPHRS)
Constraint on the design variables:	$0.45 \leq$ RMOXG2C ≤ 0.47 $0.445 \leq$ RSTM2OX ≤ 0.455 $0.80 \leq$ XSLCNV ≤ 0.95 $0.50 \leq$ SCRAE ≤ 0.90 $5.0 \leq$ XNH3S ≤ 20.0 $0.5 \leq$ CF ≤ 0.9 $5000 \leq$ REPHRS ≤ 25000
Other constraint:	NO_X Emissions (For stochastic optimization, constraint is on upper 90th percentile of NO_X emissions; for stochastic programming, constraint is on NO_X emissions in each sampling iteration)

Table B-2. Optimal Solutions from Stochastic Optimization Considering Variability in Model Inputs when the 90th Percentile of NO_X Emissions is Constrained

	Level 1	Level 2	Level 3
Constraint on NO_X Emission ($lb/10^6$ Btu)	90th percentile of NO_X emissions $\leqslant 0.3$	90th percentile of NO_X emissions $\leqslant 0.2$	90th percentile of NO_X emissions $\leqslant 0.1$
Minimum expected cost of electricity (mills/kWh)	47.02	47.22	47.41
Gasifier Oxygen to Carbon Ratio	0.45	0.45	0.45
Gasifier Steam to Carbon Ratio	0.455	0.455	0.455
Sulfur retained in the gasifier bottom ash	0.95	0.95	0.95
SCR NO_X Removal Efficiency	0.54	0.70	0.86
SCR ammonia slip (ppm)	5	5	5
Plant Capacity Factor	0.9	0.9	0.9
SCR Replacement Interval (hours)	25000	25000	25000

Table B-3. Optimal Solutions from Stochastic Programming Considering Variability in Model Inputs

	Level 1	Level 2	Level 3
Constraint on NO_X Emissions ($lb/10^6Btu$)	NO_X emissions ≤0.3	NO_X emissions ≤0.2	NO_X emissions ≤0.1
Mean Value of the Optimal cost of electricity (mills/kWh)	46.99	47.11	47.35
95% range of optimal cost of electricity (mills/kWh)	45.12 ~ 49.25	45.15 ~ 49.38	45.40 ~ 49.62
Mean value of optimal RMOXG2C	0.45	0.45	0.45
95% range of optimal RMOXG2C	0.45 ~ 0.45	0.45 ~ 0.45	0.45 ~ 0.45
Mean value of optimal RSTM2OX	0.453	0.453	0.453
95% range of optimal RSTM2OX	0.448 ~ 0.455	0.449 ~ 0.455	0.448 ~ 0.455
Mean value of optimal XSLCNV	0.95	0.95	0.95
95% range of optimal XSLCNV	0.94 ~ 0.95	0.94 ~ 0.95	0.94 ~ 0.95
Mean value of optimal SCRAE	0.51	0.61	0.81
95% range of optimal SCRAE	0.5 ~ 0.62	0.5 ~ 0.74	0.71 ~ 0.88
Mean value of optimal XNH3S	7.2	8.4	8.6
95% range of optimal XNH3S	5 ~ 10.6	5 ~ 15.6	5 ~ 17.8
Mean value of optimal CF	0.9	0.9	0.9
95% range of optimal CF	0.9 ~ 0.9	0.9 ~ 0.9	0.9 ~ 0.9
Mean value of optimal REPHRS	24765	24730	24803
95% range of optimal REPHRS	23963 ~ 25000	23550 ~ 25000	23940 ~ 25000

Table B-4. Comparison of Stochastic Optimization and Stochastic Programming Results when Variability in Model Inputs is Considered

	Level 1	Level 2	Level 3
Stochastic Optimization Results			
NO_X emission constraint	Probability (NO_X emissions ≤ 0.3) ≥ 0.90	Probability (NO_X emissions ≤ 0.2) ≥ 0.90	Probability (NO_X emissions ≤ 0.1) ≥ 0.90
Minimum expected cost of electricity	47.02	47.22	47.41
SCR Removal Efficiency	0.54	0.70	0.86
Stochastic Programming Results			
NO_X emission constraint	NO_X emissions $\leqslant 0.3$	NO_X emissions $\leqslant 0.2$	NO_X emissions $\leqslant 0.1$
Mean value of cost of electricity	46.99	47.11	47.35
Mean value of SCR removal efficiency	0.51	0.61	0.81
Expected Value of Perfect Information (EVPI) *			
Mills/kWh	0.03	0.11	0.06
10^6\$/Year	0.18	0.66	0.36

*: for Level 1: EVPI is calculated as the difference between the optimal expected cost of electricity from stochastic optimization in which 90th percentile of NO_X emissions is constrained to be less than or equal to 0.3 lb/10^6Btu, and the average optimal cost of electricity from stochastic programming in which NO_X emissions are constrained to be less than or equal to 0.3 lb/10^6Btu. EVPI for Level 2 and Level 3 are calculated in the same way.

Optimization when Considering Uncertainty in Model Inputs

Table B-5. Formulation of the Optimization Problem when Uncertainty in Model Inputs is Considered

Configuration of the IGCC system:	Configuration 2: Gas Turbine with pressure ratio of 15.0 and turbine inlet temperature at 2350K, with Selective Catalytic Reduction (SCR)
Objective:	Minimization of Cost of electricity (mills/kWh) (For stochastic optimization, objective is minimization of expected value of cost of electricity; for stochastic programming, objective is minimization of cost of electricity at each sampling iteration)
Design variables:	1.Gasifier Oxygen to Carbon Ratio (RMOXG2C) 2.Gasifier Steam to Carbon Ratio (RSTM2OX) 3.Sulfer retained in the gasifier bottom ash (XSLCNV) 4.SCR NO_X Removal Efficiency (SCRAE) 5.SCR ammonia slip (XNH3S) 6.Plant Capacity Factor (CF) 7.SCR Replacement Interval (REPHRS)
Constraint on the design variables:	$0.45 \leq$ RMOXG2C ≤ 0.47 $0.445 \leq$ RSTM2OX ≤ 0.455 $0.80 \leq$ XSLCNV ≤ 0.95 $0.50 \leq$ SCRAE ≤ 0.90 $5.0 \leq$ XNH3S ≤ 20.0 $0.5 \leq$ CF ≤ 0.9 $5000 \leq$ REPHRS ≤ 25000
Other constraint:	NO_X Emissions (For stochastic optimization, constraint is on upper 90th percentile of NO_X emissions; for stochastic programming, constraint is on NO_X emission in each sampling iteration)

Table B-6. Optimal Solutions from Stochastic Optimization Considering Uncertainty in Model Inputs when 90th Percentile of NO_X Emissions is Constrained

	Level 1	Level 2	Level 3
Constraint on NO_X Emission (lb/10^6 Btu)	90th percentile of NO_X emissions $\leqslant$0.3	90th percentile of NO_X emissions $\leqslant$0.2	90th percentile of NO_X emissions $\leqslant$0.1
NO. of random samples	100	100	100
Stopping Criteria for Genetic Algorithm	Last 200 changes less than 1%	Last 200 changes less than 1%	Last 200 changes less than 1%
Minimum expected cost of electricity (mills/kWh)	47.95	48.14	48.36
Gasifier Oxygen to Carbon Ratio	0.45	0.45	0.45
Gasifier Steam to Carbon Ratio	0.455	0.455	0.455
Sulfur retained in the gasifier bottom ash	0.95	0.95	0.95
SCR NO_X Removal Efficiency	0.51	0.67	0.84
SCR ammonia slip (ppm)	5	5	5
Plant Capacity Factor	0.9	0.9	0.9
SCR Replacement Interval (hours)	25000	25000	25000

Table B-7. Minimization of Cost of Electricity in Stochastic Programming Considering only Uncertainty in Model Inputs

	Level 1	Level 2	Level 3
Constraint on NO_X Emissions ($lb/10^6Btu$)	NO_X emissions $\leqslant$0.3	NO_X emissions $\leqslant$0.2	NO_X emissions $\leqslant$0.1
Mean Value of the Optimal cost of electricity (mills/kWh)	47.93	48.09	48.34
95% range of optimal cost of electricity (mills/kWh)	44.42 ~ 55.73	44.55 ~ 55.90	44.77 ~ 56.13
Mean value of optimal RMOXG2C	0.45	0.45	0.45
95% range of optimal RMOXG2C	0.45 ~ 0.45	0.45 ~ 0.45	0.45 ~ 0.45
Mean value of optimal RSTM2OX	0.452	0.452	0.452
95% range of optimal RSTM2OX	0.445 ~ 0.455	0.445 ~ 0.455	0.445 ~ 0.455
Mean value of optimal XSLCNV	0.95	0.95	0.95
95% range of optimal XSLCNV	0.94 ~ 0.95	0.94 ~ 0.95	0.94 ~ 0.95
Mean value of optimal SCRAE	0.50	0.64	0.83
95% range of optimal SCRAE	0.5 ~ 0.52	0.58 ~ 0.69	0.80 ~ 0.85
Mean value of optimal XNH3S	6.6	8.3	8.4
95% range of optimal XNH3S	5 ~ 13.4	5 ~ 14.3	5 ~ 14.3
Mean value of optimal CF	0.9	0.9	0.9
95% range of optimal CF	0.9 ~ 0.9	0.9 ~ 0.9	0.9 ~ 0.9
Mean value of optimal REPHRS	24800	24800	24803
95% range of optimal REPHRS	23379 ~ 25000	23858 ~ 25000	24310 ~ 25000

Table B-8. Comparison of Stochastic Optimization and Stochastic Programming Results when Uncertainty in Model Inputs is Considered

	Level 1	Level 2	Level 3
Stochastic Optimization Results			
NO_X emission constraint	Probability (NO_X emissions ≤ 0.3) ≥ 0.90	Probability (NO_X emissions ≤ 0.2) ≥ 0.90	Probability (NO_X emissions ≤ 0.1) ≥ 0.90
Minimum expected cost of electricity	47.95	48.14	48.36
SCR Removal Efficiency	0.51	0.67	0.84
Stochastic Programming Results			
NO_X emission constraint	NO_X emissions $\leqslant 0.3$	NO_X emissions $\leqslant 0.2$	NO_X emissions $\leqslant 0.1$
Mean value of cost of electricity	47.93	48.09	48.34
Mean value of SCR removal efficiency	0.50	0.64	0.83
Expected Value of Perfect Information (EVPI) *			
Mills/kWh	0.02	0.05	0.02
10^6\$/Year	0.12	0.30	0.12

*: for Level 1: EVPI is calculated as the difference between the optimal expected cost of electricity from stochastic optimization in which 90th percentile of NO_X emissions is constrained to be less than or equal to 0.3 lb/10^6Btu, and the average optimal cost of electricity from stochastic programming in which NO_X emissions are constrained to be less than or equal to 0.3 lb/10^6Btu. EVPI for Level 2 and Level 3 are calculated in the same way.

Optimization Considering Both Variability and Uncertainty in Model Inputs

Table B-9. Formulation of the Optimization Problem when Both Variability and Uncertainty in Model Inputs are Considered

Configuration of the IGCC system:	Configuration 2: Gas Turbine with pressure ratio of 15.0 and turbine inlet temperature at 2350K, with Selective Catalytic Reduction (SCR)
Objective:	Minimization of Cost of electricity (mills/kWh) (For coupled stochastic optimization and programming, objective is minimization of expected value of cost of electricity; for two-way stochastic programming, objective is minimization of cost of electricity)
Design variables:	1.Gasifier Oxygen to Carbon Ratio (RMOXG2C) 2.Gasifier Steam to Carbon Ratio (RSTM2OX) 3.Sulfer retained in the gasifier bottom ash (XSLCNV) 4.SCR NO_X Removal Efficiency (SCRAE) 5.SCR ammonia slip (XNH3S) 6.Plant Capacity Factor (CF) 7.SCR Replacement Interval (REPHRS)
Constraint on the design variables:	$0.45 \leq$ RMOXG2C ≤ 0.47 $0.445 \leq$ RSTM2OX ≤ 0.455 $0.80 \leq$ XSLCNV ≤ 0.95 $0.50 \leq$ SCRAE ≤ 0.90 $5.0 \leq$ XNH3S ≤ 20.0 $0.5 \leq$ CF ≤ 0.9 $5000 \leq$ REPHRS ≤ 25000
Other constraint:	NO_X Emissions (For coupled stochastic optimization and programming, constraint is on upper 90th percentile of NO_X emissions; for two-way stochastic programming, constraint is on NO_X emissions)

Table B-10. Optimal Solutions from the Coupled Stochastic Optimization and Programming when 90th Percentile of NO_X Emissions $\leq 0.2 lb/10^6 Btu$

	Average Value	95% Confidence Interval	95% Range
Expected Cost of Electricity (mills/kWh)	48.28	47.67 ~ 48.89	44.82 ~ 56.00
Gasifier Oxygen to Carbon Ratio	0.45	0.45 ~ 0.45	0.45 ~ 0.45
Gasifier Steam to Carbon Ratio	0.454	0.454 ~ 0.455	0.445 ~ 0.455
Sulfur retained in the gasifier bottom ash	0.948	0.947 ~ 0.978	0.945 ~ 0.95
SCR NO_X Removal Efficiency	0.719	0.715 ~ 0.723	0.669 ~ 0.751
SCR ammonia slip (ppm)	5.1	5.0 ~ 5.1	5.0 ~ 5.3
Plant Capacity Factor	0.90	0.90 ~ 0.90	0.90 ~ 0.90
SCR Replacement Interval (hours)	24997	24996 ~ 24999	24978 ~ 25000

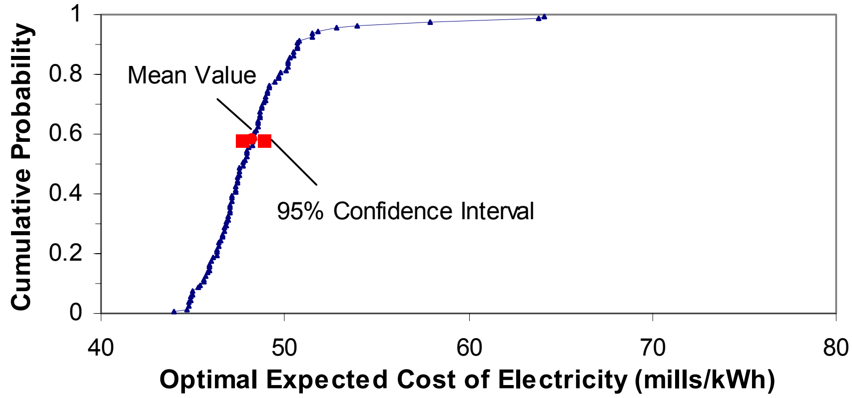


Figure B-1. Cumulative Probability Distribution for Optimal Expected Cost of Electricity from the Coupled Stochastic Optimization and Programming Method when the 90th Percentile of NO_X Emissions $\leq$ 0.2 lb/10^{6}Btu

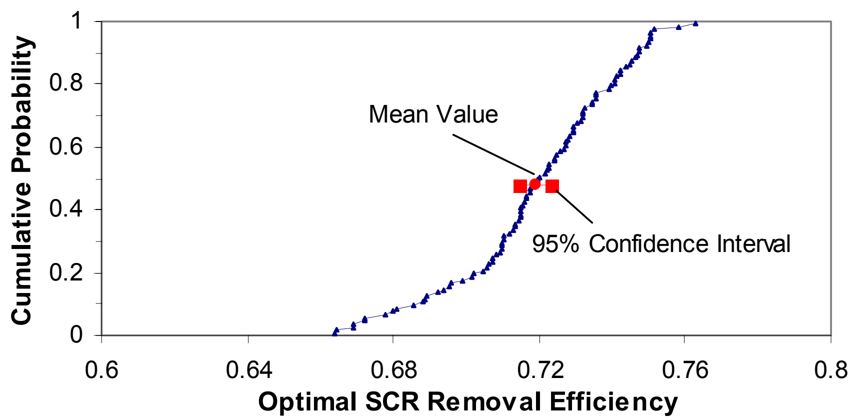


Figure B-2. Cumulative Probability Distribution for Optimal SCR Removal Efficiency from the Coupled Stochastic Optimization and Programming Method when the 90th Percentile of NO_X Emissions $\leq$ 0.2 lb/10^{6}Btu

Table B-11. Optimal Values Summary from Two-dimensional Stochastic Programming when NO_X Emissions $\leq 0.2 lb/10^6 Btu$

	Average optimal value	95% Confidence Interval
Cost of Electricity (mills/kWh)	48.16	44.60 ~ 55.99
Gasifier Oxygen to Carbon Ratio	0.450	0.450 ~ 0.450
Gasifier Steam to Carbon Ratio	0.452	0.447 ~ 0.454
Sulfur retained in the gasifier bottom ash	0.946	0.944 ~ 0.950
SCR NO_X Removal Efficiency	0.622	0.571 ~ 0.676
SCR ammonia slip (ppm)	8.37	6.84 ~ 10.49
Plant Capacity Factor	0.90	0.90 ~ 0.90
SCR Replacement Interval (hours)	24717	24471 ~ 24880

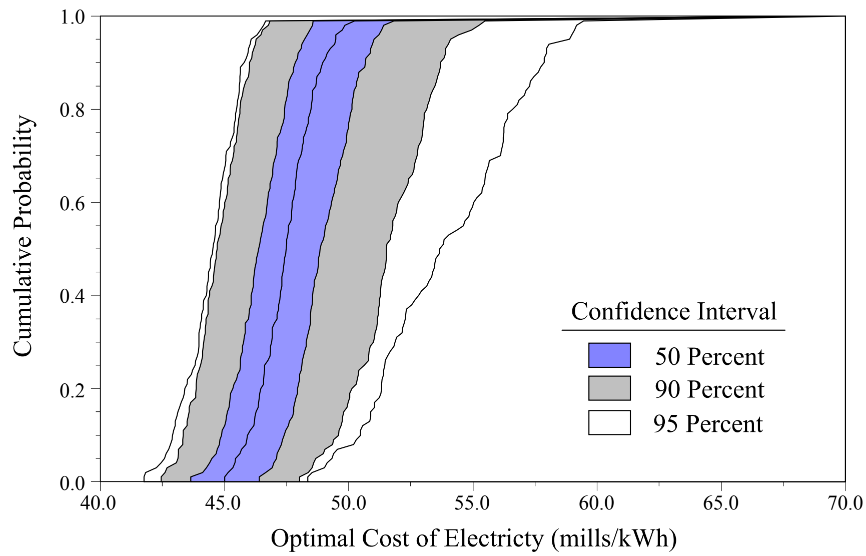


Figure B-3. Two-dimensional Distribution for the Optimal Cost of Electricity from Two-dimensional Stochastic Programming when NO_X Emissions ≤ 0.2 lb/10^6Btu

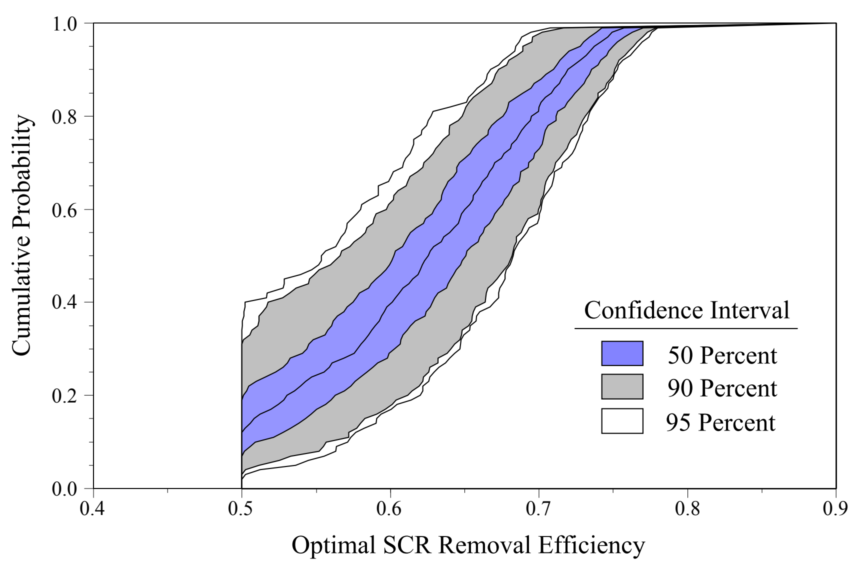


Figure B-4. Two-dimensional Distribution for the Optimal SCR Removal Efficiency from Two-dimensional Stochastic Programming when NO_X emissions ≤ 0.2 lb/10^6Btu

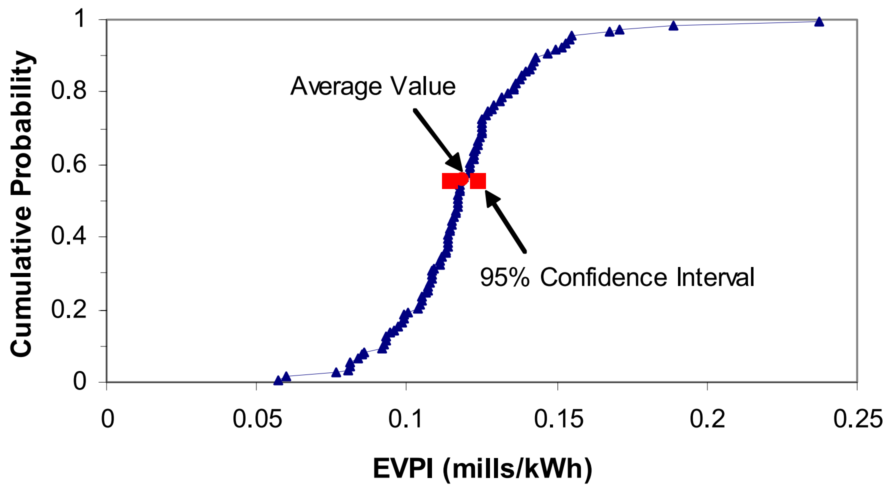


Figure B-5. Cumulative Probability Distribution of Expected Value of Perfect Information *

*: Each EVPI is calculated this way: as stochastic optimization was conducted for each realization of variability in which 90th percentile of NO_X emissions is constrained by 0.2 lb/10^6Btu, and stochastic programming was conducted for each realization of variability in which NO_X emissions are constrained by 0.2 lb/10^6Btu; One EVPI was calculated for each realization of variability. Since 100 realizations of variability were sampled, 100 values of EVPI were obtained, which can be used to construct the probability distribution shown in the figure.