To the Graduate Council:

I am submitting herewith a dissertation written by Kent Alan Williams entitled "A Methodology for Economic Evaluation of Process Technologies in the Early Research and Development Stages." I have examined the final copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Chemical Engineering.

John M. Holmes, Major Professor

We have read this dissertation and recommend its acceptance:

Accepted for the Council:

The Graduate School

A METHODOLOGY FOR ECONOMIC EVALUATION OF PROCESS TECHNOLOGIES IN THE EARLY RESEARCH AND DEVELOPMENT STAGES

A Dissertation

Presented for the

Doctor of Philosophy

Degree

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Kent Alan Williams

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ABSTRACT

A systematic methodology has been developed by the author for building, combining, and exercising a set of specially devised performance, design, and cost models in a form suitable for process economic assessments in the presence of major technological uncertainties. This document describes the development and utilization of the new methodology, i.e., one that incorporates model development and uncertainty analysis for the projection of potentially competitive, full-scale performance and costs of first-of-a-kind process technology still in the early research and development stages. Via simulation, a cohesive spectrum or distribution of the resulting performance and cost figure-of-merit values, along with their associated probabilities, is calculated.

The appropriate format for development of the user's modeling system, which includes the capability to reoptimize the proposed process for each set of process inputs considered is presented, along with the required stepwise approach for selection of values and ranges of the major uncertain process variables or inputs. The basic principles of this combined methodology can be applied to many new processes or technologies--particularly those in their early R&D stages.

Interpretation of the probabilistic output data is also discussed. Such data can be useful to the experimentalists as well as to those decision makers who must recommend or decide whether a particular process should be further developed, or which of several competing technologies should be selected for continued support.

Recent experiences with this methodology in the assessment of advanced uranium isotope separation processes and in assessment of a

photochemical syngas cleanup system allow two major conclusions to be drawn. These are (1.) that disappointments in process-performance related areas rather than hardware cost issues tend to have the most deleterious effects on unit cost and (2.) that the process proponent's earliest single-point "best guess" unit cost estimates are usually found to fall in the most optimistic fringes of the computed uncertainty ranges.

A simplified analysis of a catalytic plug flow reactor system and a highly detailed analysis of a proposed photochemical syngas decontamination process are presented to illustrate application of the methodology.

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CHAPTER I

INTRODUCTION

The Economic Assessment Problem

The Need for Improved Economic Prediction

Pressures of foreign competition, particularly in the high-technology area, the need for increased productivity, and the increasing emphasis on military and energy security have all resulted in new demands for earlier and more accurate assessments of innovative but still immature technologies.[1] With obviously limited resources, difficult selections among competing early research projects for more expensive development, scale-up, and potential commercialization are unavoidable.

Considerable private and government capital is being channeled into research and development (R&D) and scale-up efforts, oriented toward modernization of existing capital facilities and commercialization of new technology. Eventual failure or success of a productive enterprise may depend upon how well a new large-scale project meets its previously predicted performance and cost goals. For this reason it behooves R&D planners and strategic planners to obtain comprehensive and accurate projections of project performance and economics starting as early as possible in the R&D program--certainly before commitments are made for further development, scale-up, or the construction of a full-scale facility.

Effective economic assessment is also of use to R&D managers and the development community in other ways; i.e., directing resources

toward technology areas which have high economic leverage, benchmarking the progress of an R&D program toward performance and cost goals, and screening out R&D programs with low economic potential in a funding-limited environment. The decision-maker and strategic planner also need the results of economic assessment to better evaluate enterprise-related factors such as the possible effects of a new technology on process deployment strategy, future cash flows, market penetration and pricing, and competitive, overall business performance.

Example Situation: Early Assessment Needs in Uranium Enrichment

The uranium enrichment business is a production enterprise owned by the U.S. Government through the Department of Energy and operated by contractors. It is essentially a service business which enhances the isotopic uranium-235 content of uranium fuel for nuclear power reactors. Recent economic conditions, public opposition to nuclear power, foreign competition, and soaring costs have reduced considerably the orders for nuclear power plants and for the uranium enrichment service; however, the present position[2] of that enterprise still furnishes an excellent example of an industry where new innovations and technological strides have a chance of making a major impact on the competitive strength and economic health of a multibillion-dollar operation.

In recent years, several unique high-technology processes have been suggested to supersede the power-intensive and hence relatively expensive gaseous diffusion process. (Gaseous diffusion has been utilized for uranium enrichment since World War II.) These new processes were projected to incur enriched uranium production costs at a fraction of

those for gaseous diffusion, but each carried with it the need for a long, expensive development program. Since physical facilities of the magnitude of enrichment plants take at least five years to construct and require considerable R&D prior to a deployment decision, an urgent need for more systematic and accurate prediction of technology performance and costs became apparent.

The strategic planner, supplied with good estimates of future production costs, can evaluate how the projected lower unit costs of enrichment services might decrease the price eventually charged to utility customers and thereby improve the U.S. position in the world enrichment market. Expected present worth, cost/benefit ratios, and other payoffs for the new technologies can then be calculated and compared.

The managers of development programs in uranium enrichment can also redirect their program efforts toward those processes within a given mission or those R&D areas within a given process which have the greatest potential for economic success.

Some exploration of different isotope separation processes has been carried on since the World War II (Manhattan Project) days. In the late 1950s, work on the gas centrifuge process was resumed. In the 1960s and 1970s it became apparent that progress on this process and other "advanced isotope separation" (AIS) processes involving lasers or plasmas had created new and potentially more attractive options for commercial development and scale-up. The need to evaluate and select specific processes for intensified further development and scale-up

stimulated new interest in more systematic and accurate assessment methodologies.

In recent years the author has been fortunate in being given the opportunity to participate in the development of improved economic evaluation methodology. His role and contribution will be outlined in a subsequent section of this chapter. The methodology is capable of predicting the cumulative effects of identifiable technological uncertainties on the cost and performance of immature processes. This approach involves the construction of specific process models and appropriate application of a simulation technique. The presentation of these procedures is the subject of this dissertation.

The successful use of such methodology in the uranium enrichment area suggests many other technology-intensive processes for potential application. First-of-a-kind energy technologies such as magnetic- or inertial-confinement fusion and solar power plants constitute possible economic evaluation areas.

Attributes of Successful Assessment Methodology

The need exists for a generalized approach to the problem of the economic assessment of new process technology, i.e., an approach which can be utilized by experimentalists, analysts, and decision makers. The need is especially great for what are often termed "new," "immature," "infant," "first-of-a-kind," "innovative," "pioneer," or "high-technology" processes. Many of these projects represent highly innovative applications of recent discoveries in basic sciences such as physics or chemistry.

Unfortunately many such first-of-a-kind process development programs are often promoted and sustained by developer optimism. Only later in the R&D program or upon deployment or commercialization is it found that performance has fallen short of predictions, while costs exceed them.

A successful methodology capable of dealing with this problem must

1. Minimize potential biases in projections.
2. Be applicable at early stages of R&D when uncertainties abound.
3. Make use of limited data that are obtainable.
4. Require a reasonable level of effort.
5. Be understandable and useful to technologists and strategic planners.

For first-of-a-kind technologies in the early R&D stages, on which this methodology if focused, the three keys to successful economic evaluation will be seen to lie in collection and careful analysis and structuring of the available pertinent facts and data, comprehensive process modeling, and proper use of statistical uncertainty concepts.

Specific Application of Methodology to the Evaluation and Selection of Advanced Isotope Separation Processes

Simultaneous advancement of both laser technology and plasma physics resulted in significant R&D work on highly innovative advanced isotope separation (AIS) methods for the uranium enrichment step of the nuclear fuel cycle. By 1976, three AIS processes were being funded by the Department of Energy: the Molecular Laser Isotope Separation (MLIS) Process, developed by Los Alamos National Laboratory; the Atomic Vapor

Laser Isotope Separation (AVLIS) Process, developed by Lawrence Livermore National Laboratory; and the Plasma Separation Process (PSP), developed by TRW Incorporated. All three of these processes involved high-technology hardware still in the basic laboratory stages, and each had been demonstrated on the proof-of-principle level. A number of the key scientific and cost issues relevant to scale-up of these processes were highly uncertain or left to be determined--hence, the need for inclusion of economic assessment suitable to these conditions as an activity conducted in parallel with R&D.

By the late 1970s, budgetary considerations dictated that DOE choose only one of these three processes for further R&D. Each contractor laboratory was asked to explore and contribute certain critical basic information on its proposed process candidate. The Union Carbide Corporation-Nuclear Division (UCC-ND) at Oak Ridge was assigned the task of modeling and assessing the technical and economic aspects of the three proposed AIS processes. The general methodology developed and here described played a key role in the May 1982 DOE Headquarters decision to choose the AVLIS process for further engineering and development. The fact that this methodology played such an important role in an $80-million-per-year government program decision is documented in the Congressional Record.[3]

In these process assessment and selection efforts, which involved the development of special process models and their Monte Carlo treatment for uncertainty analysis, the author was responsible for development of the initial process performance model for the AVLIS process described above and the development of economic models for all three AIS

process contenders. For computer simulation purposes the Monte Carlo technique was applied to the uncertainty evaluation at the suggestion of Richard L. Hoglund. He had become acquainted with Hertz's[4] application of the technique to economic and business analysis and projections. The author had been aware of analogous applications in the simulation and prediction of the behavior of highly uncertain or random physical systems. It soon became apparent that with the correct modeling and data-gathering approach, the Monte Carlo method could be utilized in the assessment of many processes where technical uncertainties abound.

Monte Carlo analysis techniques are not new, and their historical use is well documented.[5] Eighty years ago Lord Kelvin developed such techniques for his study[6] of the Boltzmann equation utilized in statistical mechanics. More intense use of the techniques began as part of the Manhattan Project during World War II, mostly in the course of studies of the physics and design of the atomic bomb. For example, Von Neumann and Ulam[7] utilized the method to simulate neutron diffusion in fissile material for this weapons application. Since then the Monte Carlo method has been utilized in nuclear reactor design, plasma physics, and many other research applications. As stated its first use in the area of economic enterprise (1964) was that of Hertz for analysis of marketing uncertainties.[8] Availability of high-speed digital computers made feasible the application of Monte Carlo techniques to a wide range of scientific, engineering, and operations research problems.

Tasks, Models, and Figures of Merit for Early Economic Evaluations

In the appraisal of development projects for eventual deployment there are two important classes of uncertainties which must be considered. Technological uncertainties are those process related hardware cost, design, reliability, and performance uncertainties which impact the productivity and capital and operating costs of a proposed facility. Strategic uncertainties are those related to project finance, the timing of development, deployment, and construction, and the state of overall enterprise and economy under which the project would be deployed. Both types of uncertainties are important to any figure of merit utilized in economic evaluation; however, if an overall economic assessment effort is subdivided into three parts or tasks, it can be seen that particular classes of uncertainties, types of models, and figures of merit are appropriate to each task.

Each of the three tasks may have its own modeling tools and each attempts to answer a different set of questions. Figure 1.1 shows the tasks, data requirements, and figures of merit schematically.

The development planning task (I) has as its figure of merit the dollars which must be spent to resolve a set of technological issues in sufficient time that the process can meet a given (but perhaps uncertain) deployment goal. Uncertainties in both timing and technology development requirements would have to be considered by such a model. Several decision analysis modeling packages for development planning tasks are currently available and with the proper input data can be utilized for numerous types of development projects.

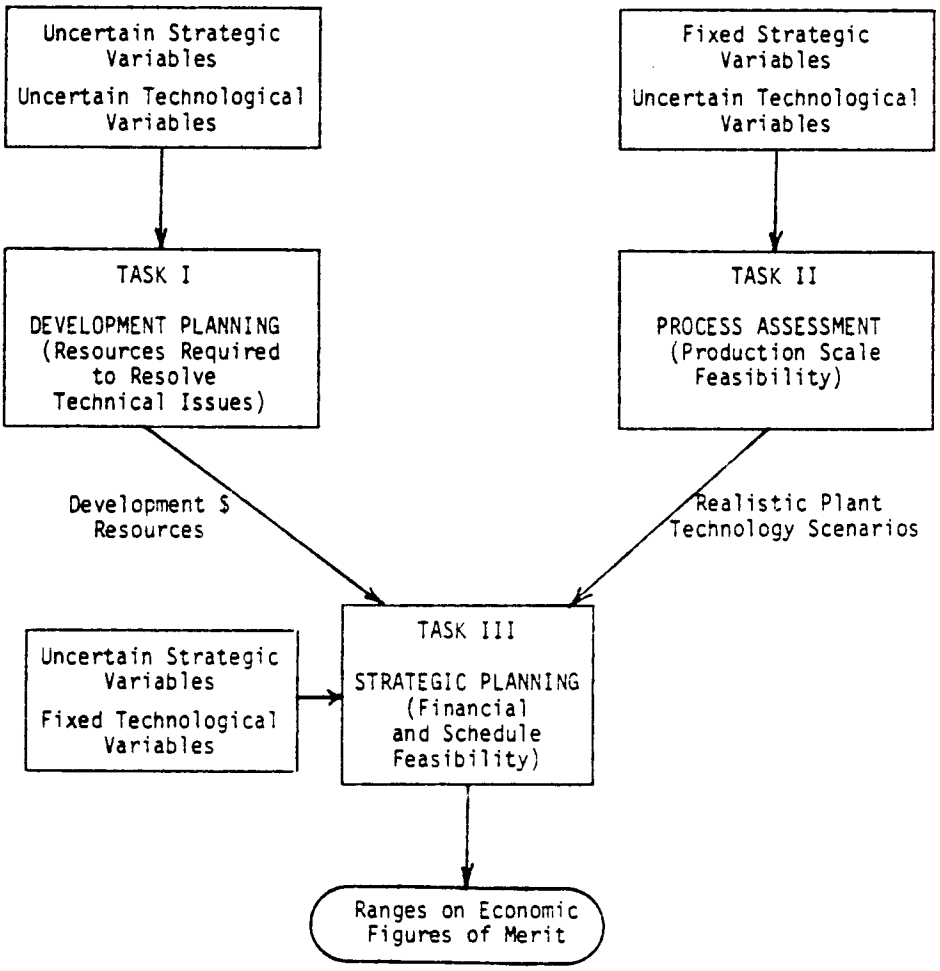


Figure 1.1

The Three Economic Evaluation Tasks for Processes in Research and Development

The process assessment task (II) has as its goal determination of the effects of technological uncertainties on the productivity, capital costs, and operating costs of a hypothetical production facility. In order to perform this task, one must assume "best guess" values for strategic variables, such as interest rate, construction time, production campaign length, and product demand. By fixing these strategic variables, i.e., not considering their uncertainties simultaneously with technology uncertainties, one can distinguish more readily the cost driving effects of technology issues alone. For this analysis task figures of merit might be capital costs, operating costs, unit costs, rate of return, or others more appropriate to the analyst's project. In order to perform this task, process specific models are required. For processes in the early development stages this task is extremely important, and the methodology discussed in this dissertation will address predominantly this second task.

The strategic planning task (III) predominantly considers uncertainties related to both development and production facility timing issues, financing considerations, and the production enterprise and national economy as a whole. This task is essentially the converse of task II in that the technology variables are fixed to "best guess" values such that the effects of the strategic variables can be separately examined. The figures of merit are most likely to be financial, such as rate of return or payback period; however, some may be the same as those for task II. The model which considers strategic issues must be enterprise or process specific and will be different than those models utilized for tasks I or II; however, output data from tasks I and

II will be required as input to task III. The application of uncertainty analysis to this type of model considered by task II is essentially the use of the Monte Carlo technique suggested by Hertz[9] for investment analysis.

It should again be noted that this dissertation considers mainly the second (technological uncertainty) task. For handling the task II analysis of technological uncertainties related to plant feasibility, the unit cost of product is a useful figure of merit, since it incorporates both process productivity and cost. For the examples utilized in this document, the unit cost will be the utilized figure of merit, since the cost and performance effects of technology are the predominant emphasis. Strategic variables may be equally important uncertainties. However, significant documentation of methods for analysis of their uncertainties already exists, hence they are not considered in detail in this work. It should be noted, however, that simulation can be used for calculating the uncertainty in any figure of merit, including ones dependent on the development and deployment schedule. The issue of the plant deployment schedule and its effects on process economics (Task III) will be only briefly considered in Chapter IX.

Purpose of Dissertation

A need exists for a systematic economic evaluation methodology for new process technologies. One such methodology was developed to assist DOE-funded activities for the evaluation of uranium enrichment technology. Based on this experience, the author will develop, outline, and illustrate the methodology. It is uniquely and particularly suitable

for predicting the combined effects of estimated technological characteristics and costs, as well as their uncertainties, on the competitive future, full scale performance of presently still immature processes in the early R&D stages.

One particular proposed high technology process, the use of laser photochemistry for the removal of low concentrations of sulfur from synthesis gas feedstocks used in methanol production plants,[10] is subjected to the methodology described. This particular process does not relate to aspects of national security as do the uranium enrichment technologies, hence it can serve as an unclassified example and can be discussed in more specific detail.

The next chapter, Chapter III, summarizes this assessment methodology and the contribution it can make to the state-of-the-art of economic evaluation as a branch of chemical or process engineering. Individual functions and steps in the evaluation methodology are then further described in the subsequent chapters.

CHAPTER II

SUMMARY

Prior State-of-the-Art

Because of the magnitudes of the costs, potential benefits and risks involved, projections of plant performance and costs are almost continually updated throughout the various research and development stages of major new technologies or processes. From past experience, such projections generally overestimate the subsequent actual production-scale performance and underestimate the actual capital and operating costs. It may not be too surprising that the earliest estimates exhibit the greatest degrees of deviation in this regard.

The tendency toward forecasting biases is aggravated by the application of relatively conventional cost and performance assessment techniques to immature, new, or first-of-a-kind processes. In the conventional approach to economic assessment a single, "best-guess" set of process performance and cost estimates is developed for a single process design. At times "optimistic" and "conservative" sets are also developed on a somewhat arbitrary, judgmental basis. They are generally presented to illustrate awareness of uncertainties; however, there is no systematic approach for their development and use, and usually the planning is still based on the "best-guess" set of calculated figures of merit.

The major weakness of this method is that even the most crucial technological uncertainties may not be systematically factored into the performance and cost estimates. Particularly for a process or

technology in the early stages of research and development, there are many major scientific and engineering uncertainties and unknowns which should be superimposed on the estimating uncertainties that are usually associated with scale-ups to production facilities. Many of these vaguely treated or untreated uncertainties can later turn out to be critical to the ever-present "proceed with development" versus "stop development" decision.

A systematic approach to the factoring of uncertainties into forecasts for R&D projects has the advantage of forcing an opening of the minds of the project developers. This tends to (1) counteract the natural early biases and (2) encourage greater attention to all of the critical variables and parameters upon which the ultimate performance and competitive success of the new process will depend.

The Review of the Literature in the next chapter (Chapter III) describes the past attempts of several authors to understand, document, and correct the misestimation problem for both conventional and new and still immature process technologies. Some of these attempts were based on the hope that certain standardized correction factors, derivable from experiences encountered with several past R&D projects and their process characteristics, could be used simply to correct the projections of the full-scale performance and costs of similar or analogous new R&D projects. Although sound methods of regression analysis were used to develop these factors, the cases examined were representative of only a limited class of fairly well-defined process technologies.

In Chapter III there is also a discussion of how David B. Hertz[9] analyzed highly uncertain complex business planning situations or

systems in which new technologies do not constitute the key sources of uncertainties. In 1964 he systematically applied the by then well established Monte Carlo technique to the financial analysis of technologically proven commercial ventures with uncertain market size, selling price, market share, and required investment.

Improvement to the State-of-the-Art

In the approach presented in this dissertation, process specific models of estimated full-scale performance and costs, including probabilities, are developed and exercised by means of the Monte Carlo simulation technique. This new method of techno-economic assessment is particularly applicable to major new-technology or new-process R&D. This emphasis in application also leads to considerable need for new methodology which will be presented and discussed in reference to certain actual and illustrative process analyses.

Recently, the Department of Energy has been faced with the task of assessing three radically different and still immature, competitive uranium isotope separation technologies. It soon became apparent that the conventional techniques of economic analysis normally utilized for much better-known technologies such as oil refineries, chemical plants, and electric power plants were not applicable.

In the ensuing competition among the processes for continuing funding and survival at the time, the key concerns and questions were not associated with uncertainties in demands, pricing, and deployment strategy. Rather, the main questions were: how well will each of the competing infant technologies work and produce, and how much is it

likely to cost to build and operate plants of comparable desired productivity? In other words, what will be the competitive, full-scale unit cost of product? To make matters even more complicated, the processes were scientifically very complex and had to rely upon untried basic technologies, such as the development and scale-up of high-power lasers and applications of plasmas, applied to production processes.

Because of the great variety of process complexities and uncertainties, it soon became apparent that the construction of comprehensive mathematical models would be virtually unavoidable. Only such models could incorporate and track the basic science and engineering knowns and unknowns of the three processes and allow the analysts and management to arrive at sound, common understanding of the combined critical performance and cost issues, and their uncertainties and implications.

Furthermore, the Monte Carlo method was deemed to be applicable to the consistent treatment of such mathematical process models.

The new procedure starts with careful modeling of all significant technological steps and cost-related factors. This is followed by the application of the Monte Carlo technique for uncertainty analysis. By this approach, which can utilize early and sketchy theoretical and experimental discoveries, along with peer review techniques, it becomes possible to generate ranges and probabilities for the performance and cost-related figures of merit of each process. Consequently, the results are much more comprehensive and useful than those stemming from any oversimplified comparisons among single-point or three-point (best-guess, optimistic, and conservative) estimates.

Initially, because of the inadequacies in the earliest models, qualitative adjustment factors were used for some figures of merit.

The basic approach to process assessment will be described further and illustrated in the following pages. It should be noted that it requires the development of an assessment model consisting of performance, design, and cost-scaling modules for each new process.

For conventional chemical engineering technologies such as refineries, petrochemical plants, and fertilizer plants, this methodology has limited usefulness. Uncertain process performance is usually not the major issue, and well-documented cost information is likely to be available. Chemical technology, however, is branching out into many high technology areas such as photochemistry, biochemical engineering, new applications of electrochemistry, and production of synthetic fuels where uncertain process performance questions are likely indeed to constitute dominant issues. Thus, this document should be of primary use to the chemical or process engineer who must assess these new types of technologies and processes. They should have the best knowledge of the process attributes which drive both performance and cost. In essence, this document is intended to serve as a guide for the assessment team as well as the competing experimental project teams, and, of course, their common management.

Outline of Approach Methodology and Subsequent Chapters

The following subsections of this summary outline the approach to the process assessment, as well as most of the remaining chapters of

this dissertation. The same sequence and structure is also illustrated in Figure 2.1.

As indicated previously, the next chapter (Chapter III) contains a review of the prior literature.

Chapter IV is intended to assist the user in determining whether a particular R&D project fits the conditions for application of the techniques described here. A two-way test is applied to the project to ascertain (1) whether basic new-technology or new-process uncertainties are involved, and (2) how well the particular R&D project is suited for analysis under the evaluation procedure developed in this document?

Once applicability of the methodology has been established, most of the remaining chapters (Chapters V through IX) are intended for use in the actual assessment task.

Chapter V outlines the particular technique which the user can follow in assessment model construction. The particular performance, design, and cost modules will of course have to be developed by the user on a process-specific basis. Mathematically the combined performance, design, and cost-scaling model forms a complex "transfer function" with which one must be able to calculate the performance, design, and cost consequences of variations in one or several of the major independent process input variables. The triggering event or forcing function in this case would be a change in one or more of these major inputs dictated by new experimental results, a development breakthrough or disappointment, improved theoretical calculations, or by any newly encountered uncertainties or unknowns.

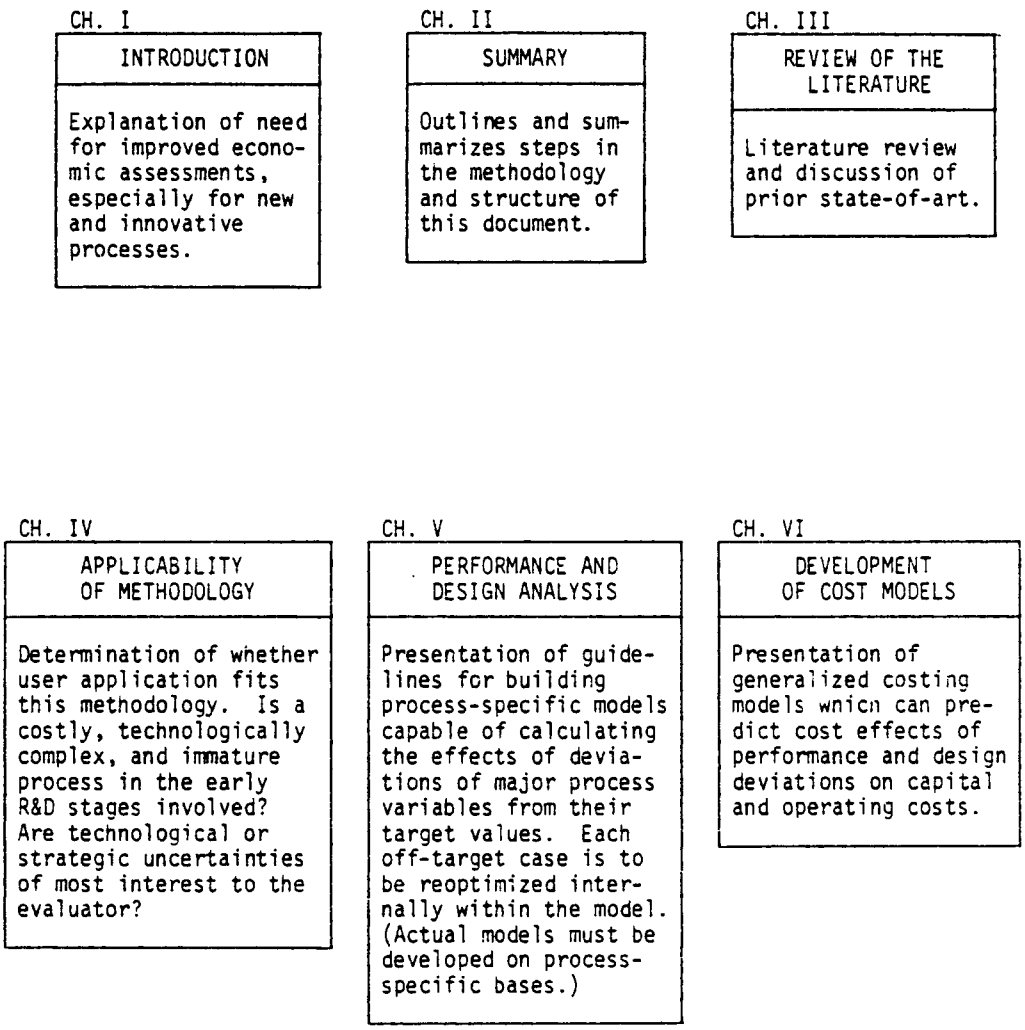


Figure 2.1

Summary of Economic Assessment Methodology for Immature Process Technologies in the Early R&D Stages

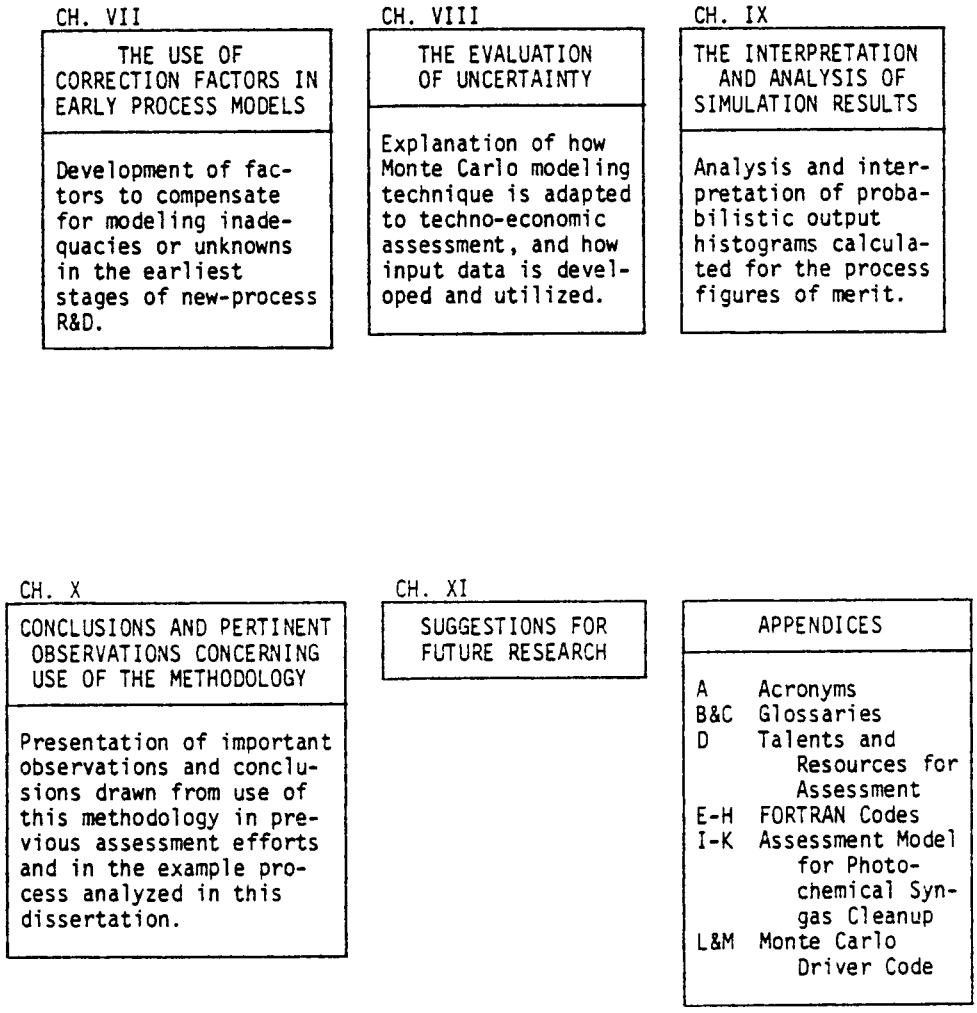


Figure 2.1 (Continued)

Irrespective of the specific combination of deviations in the major input variables, the model itself must be able to reoptimize and redesign the process to restore its target performance or productivity for each assumed case or combination. The model performs the redesign task and projects responses, i.e., altered figures of merit such as the capital cost and the unit cost of product.

Also distinguished from prior state-of-the-art is the use of a computer model for the required repetitive process reoptimization and redesign. The model should be capable of the rapid generation of widely ranging figures of merit for the many cases or combinations considered. When many major input variables are involved, a manual design team approach, in which hand calculations are involved, would be too time-consuming and costly.

It has been the author's experience that the deviation/transfer function/response format and the exercising of this performance, design, and cost model are amenable to the Monte Carlo uncertainty evaluation technique. The necessary techniques for performance and design modeling, along with an example of the required algorithmic forms, are also presented in Chapter V.

Chapter VI deals with cost scaling. Cost scaling principles are somewhat less process-specific; therefore, a more detailed computer coding framework applicable to a wide range of new processes is also provided. Generally useful algorithms are presented for the calculation of process capital costs, estimating allowances, operating costs, and unit production cost. The important role of the reliability of process components is also discussed, and reliability algorithms are developed.

A FORTRAN-based cost model which includes examples of such algorithms is also presented. With appropriate user-supplied data and slight adaptations, it should be applicable for many new technologies or processes in the early R&D stages.

Chapter VIII describes how correction or adjustment factors can be occasionally developed and applied to the computed figures of merit. Such correction factors should be used only in the earliest user-constructed models and only to account for modeling inadequacies. These factors rely heavily on user judgment, thus they have the disadvantage of uncalibrated subjectivity.

Adaptation of the Monte Carlo uncertainty-evaluation technique and its combination with the overall performance, design, and cost-scaling models is discussed in Chapter IX. In addition, Chapter IX outlines the procedure for the selection of appropriate input variables, the heuristic processes involved in determining their range of values, and development and use of the proper probability distributions. A FORTRAN-based Monte Carlo simulation code is used for the actual uncertainty calculation. It operates by calling upon the process assessment model (performance, design, and cost modules) as subroutines.

Chapter X guides the user through interpretation and use of the results, i.e., the probabalistic output data, obtained from application of the techniques described above. For example, one must establish the most critical uncertainties of each process and ascertain its readiness for the next stage of research and development. The problems likely to be encountered in comparing results for two or more competitive

processes are also discussed. The evaluator's attitude toward risk is also placed in context and shown to be important.

Chapter XI presents additional, potentially useful observations and conclusions, based on recent experiences in applying this methodology. Most important may be the experience that unexpected imperfections or inefficiencies in performance, rather than underestimated component costs, are likely to be the predominant sources of unit cost underestimation in the early R&D stages. Inability to achieve the predicted performance (due to shortfalls in component performance) forces the assessment model to specify additional or larger-size equipment, which in turn increases the capital and total unit cost of product.

It is another important observation that the usual developer-generated, best guess (single-point) estimate of unit product cost falls in the optimistic (low unit cost) portion of the calculated uncertainty range. Accordingly, use of this methodology tends to compensate for the inherent biases which result from natural developer optimism, enthusiasm, and perhaps a bit of salesmanship. Experience has also shown that the proposed approach helps greatly in focusing the research and development program's efforts on the most important process performance, design, and cost issues and their successful resolution in the course of further R&D.

Chapter XII contains suggestions for further research in this area. As additional first-of-a-kind processes are subjected to this type of analysis, and as they are fully developed and deployed, an historical data base will be gradually augmented. This would also facilitate the

derivation of more applicable correction factors for subsequent new processes--especially in the early phases of their R&D.

Several appendices are attached to aid the user in more detailed aspects of the methodology. Among these are:

1. A brief discussion of the talents and support resources required for intensive and continuing techno-economic process assessment. (Appendix D)
2. An illustrative, complete, and detailed analysis for a suggested process: photochemical sulfur removal from synthesis gas feedstock. (Appendices I, J, and K)

Application of the Methodology to a Photochemical Process

Each of the six analytical steps (represented by Chapter V-X) are applied to the photochemical method in Appendices I, J, and K. The applicability criteria presented in Chapter IV indicate that this process is highly suitable for use of this methodology. The photochemical syngas cleanup method was proposed in a paper[10] by researchers at Lawrence Livermore Laboratory.

For the Chapter V step (Performance and Design Analysis) a performance and design model is developed which specifies the optimal laser power and sulfur collector size for a given set of physics and chemistry parameters submitted to the model. The annual amount of syngas decontaminated and the extent of decontamination (98% removal of the sulfur entering the chamber) are held constant. Solution of a differential equation relating conversion (percent of H_2S photodissociated) to the laser power and photochemical reactor operating conditions is required.

The Chapter VI step (Development of Cost Models) involves the development of cost scaling algorithms for the major hardware and support facilities required to implement the photochemical process. Among the equipment items scaled are the photolytic reactor (a nozzle), the laser system and its optics, a power recovery system, sulfur collectors, compressors, piping, instrumentation, utilities systems and a process building. Capital costing allowances and annual operating costs are also considered. The main figure of merit is dollars per ton of methanol produced from the decontaminated syngas feedstock.

For the Chapter VII step (Correction Factor) use is made of correction factors to adjust capital costs and productivity. These factors are applied for illustrative purposes only in this case and are not necessarily indicative of real modeling deficiencies.

For the Chapter VIII step (Evaluation of Uncertainty), twelve uncertain input variables are identified and utilized in the simulation of the photochemical process. The rationale for their selected ranges and statistical parameters is discussed in detail in Appendix I. Five hundred sets of non-target input variable values are submitted to the assessment model and frequency histograms are constructed for several figures of merit, including total and incremental cost per ton of methanol, laser output power, capital costs, and photon costs.

The results of the analyses indicate that the photochemical process proponents greatly underestimated the cost that a photochemical sulfur removal process would add to the cost of producing methanol from syngas. Their original calculation indicated only a $1.60 increase in MeOH costs per ton over the $176/ton cost for methanol produced with no prior trace

sulfur removal. The baseline single point "best guess" value obtained by use of the assessment model presented in Appendix J indicates a $25/ton unit cost increase ($201/ton MeOH). This increase is largely a result of the assessment model considering hardware costs and annual operating costs not included in the proponents "very preliminary" calculations.[10]

When uncertainty analysis is performed, the mean value for the methanol unit cost calculated from the output frequency histogram is found to be $227/ton MeOH. Overoptimism in the selection of "best guess" values for performance related input variables accounts for most of the additional increase over the $201/ton baseline above. The uncertainty in hardware cost input variables contributed only marginally to the unit cost uncertainty. Calculation of conditional probabilities indicated that the standard deviation in the unit cost frequency histogram attributable to performance uncertainity was a factor of 17 higher than that attributable to hardware cost uncertainty. Table 2.1 summarizes the analysis results for this process.

These results for the photochemical process, along with similar results experienced in the analysis of advanced isotope separation processes, support the two conclusions presented in Chapter X and are discussed in detail in Appendix I.

New Demands on Economic Evaluation Methodology

This document represents the author's synthesis of experience and methodology acquired over several years of project and process assessments. The Department of Energy's mission to fund high technical

Table 2.1

Comparison of Single Point and Probabilistic Unit Cost Results for Photolytic Syngas Example

Case Description	Range on Unit Cost* (5-95 percentiles)	Mean Unit Cost*	Standard Deviation
	NO UNCERTAINTY ANALYSIS		
Single Point Unit Methanol Cost (no sulfur removal).	---	176	---
Single Point Unit Methanol Cost (photochemical S removal: proponent's preliminary estimate[10]).	---	178	---
Single Point Unit Methanol Cost (photochemical S removal: "best guess" values of input variables supplied to assessment model).	---	201	---
	UNCERTAINTY ANALYSIS		
All 12 uncertain variables	196-306	227	40
Performance related variables are uncertain. Hardware cost variables fixed at "best guess" values.	196-295	224	38
Hardware cost related variables are uncertain. Performance cost variables fixed at "best guess" values.	201-209	206	2.3

*Unit Cost in $/ton of Methanol.

risk energy technology and its need to track development progress are are essentially the raison d'etre for this advancement in the state-of-the-art of chemical engineering--and particularly the R&D planning, process selection, and design phases of chemical engineering.

Obviously, new technologies are amenable to a variety of methods of analysis rather than a single technique. It does seem, however, that the last decade or two has brought a requirement for the more rapid development of complex, first-of-a-kind technologies from the basic discoveries to their full deployment. In this rapidly moving and highly competitive environment, a more systematic approach to the continuing evaluation and redirection of multifaceted and complex R&D from the earliest phases appears to be particularly in order. Much greater use of computers and models is also bound to be encountered in these applications.

CHAPTER III

REVIEW OF THE LITERATURE

Introduction

The nature of the problem addressed by this document is better appreciated if a review of work by others is presented. Such a summary can both provide justification for the assessment methodology and a framework against which the methodology can be judged. Since the emphasis of this work is on evaluation of production process technology, this review will deal solely with this type of project.

Basically, there are four steps which comprise a complete process evaluation: (1) projection of economic potential, (2) incorporation of uncertainties, (3) projection and assessment of technology developments via the use of pertinent available data, and (4) interpretations and use of the resulting economic projections. Each individual step can be associated with significant literature contributions; however, no single contribution treats all four steps together. For this reason the division of this section will be topical, and within each division, historical. The first division will review the literature related to why single-point economic projections (i.e., project construction or capital cost estimates) and why estimates of project performance made during R&D stages are often grossly in error. It will discuss one significant attempt to ameliorate this problem. The second will consider past efforts at incorporating uncertainty analysis in tandem with mathematical modeling. The third division considers the problem of technology

forecasting, i.e., the procedure which provides the educated judgments needed to bound the "knowns" incorporated in a modeling process. The fourth briefly relates to the interpretation of statistical data on figures of merit in situations where a decision concerning selection or deployment must be made for one or more technologies.

Should definitions of cost engineering terminology, such as the various categories of costs (capital, operating, unit, etc.), be required as the reader proceeds, a glossary is found in Appendix B.

Problems Experienced in Projecting the Economic Potential of Untried Technologies

R&D Cost Estimation Experience

Research and development on new production processes is in most cases oriented toward the eventual operation of large-scale facilities capable of competing with or ultimately replacing more conventional technology. In the early R&D stages, i.e., well in advance of a deployment decision, the basis of this competition is almost always process economics, with the figure of merit often being the product unit cost. Typical figures of merit might be dollars per kilowatt-hour ($/kW-hr) for a solar power plant or dollars per separative work unit ($/SWU) for a uranium enrichment plant.

Corporate or governmental support of such R&D frequently depends on a simultaneous economic evaluation effort which benchmarks progress toward process performance and economic goals. For this reason, throughout the development program the R&D community is often asked to prepare an estimate of probable process production costs, with typical figures of merit being unit cost of energy or other commodity produced,

rate of return (ROR), or the total estimated capital cost of a facility. Prior to the widespread use of digital computers, such evaluation efforts involved consideration of many hand-calculated cases. Buchanan[11] describes the types of calculations and data bases most chemical companies used in the past to evaluate new R&D projects and project unit production costs. These data bases did not necessarily include novel or first-of-a-kind technologies, and in most instances R&D work represented extensions of conventional chemical technology.

Experience with these more conventional chemical and energy technologies, for which process facilities are presently in operation, shows that the accuracy of early estimates, if accuracy is gauged by the difference between the estimated and inflation-adjusted experienced production costs, is usually poor. Normally, the experienced costs turn out to be significantly higher than the original early estimate. By an early estimate is meant one which is made during the R&D program but before operation of an integrated test facility, i.e., a facility in which all process steps operate simultaneously, such as a pilot plant.

An early attempt to document the problem of underestimation of the capital facility or construction cost portion of the overall production cost was presented by W. T. Nichols.[12] For conventional chemical processes an attempt was made to correlate the accuracy of an estimate with the level of information and engineering detail supporting that estimate. He found that the actual capital cost can range from 60% under to 90% over an early R&D capital estimate, even though process flow sheets and preliminary energy and material balances existed at the time of the R&D estimate.

Meadows and Marquis[13] studied the characteristics of forecasting errors in R&D project capital costs encountered by three firms producing chemical intermediates. One hundred forty-four R&D projects were studied, all of which were less than $100,000 (1968 dollars) in size. Projects which became commercial failures overran their estimated costs by factors ranging from 1.28 to 4.25. Projects which became commercially successful had factors ranging from 0.94 to 1.27. All of these projects would be very small, both in scope and funding, compared to the process technologies which would be evaluated by the methodology presented in this document.

The Rand "Pioneer Plants" Study

In the first part of a recent Rand Corporation report by E. W. Merrow et al.[14] dealing with pioneer process plant projects, the problem of inadequate capital cost estimation was discussed in detail along with possible reasons for observed differences between actual and predicted capital cost. Their results were based on the analysis of data from 44 pioneer process plants, most of which involve chemical processing. The first part of the Rand study reviewed what was known about the problem of poor capital cost and productivity estimation for pioneer technologies in particular and other very large projects in general. The study concluded that:

1. Severe underestimation of capital costs is the norm for all new technologies, and this experience is similar to the capital cost underestimation observed in weapons systems[15] and large public works projects.[16]

2. Many such projects experienced reliability and performance shortfalls. Performance is measured by Rand as the ratio of the experienced productivity to the predicted productivity.

3. Up to the time of the Rand study, only major weapons systems had been the subjects of detailed statistical analyses that successfully isolated the generic factors which contribute to the underestimation of project costs.

Shortcomings of Single-Point Estimates

It should be noted that the above literature deals with single-point capital cost estimates and their probable error ranges. Single-point estimates represent the only set of detailed information per process and correspond to only one set of input design data. Except for the inclusion of cost estimating contingencies, no attempt is made to incorporate the effect of uncertainties at the detail level. The error bands on the ratio of estimated to experienced capital costs discussed are derived from statistical analysis of many early estimates and comparing them to later experienced project capital costs after the effects of inflation are removed.

Capital Cost Estimate Accuracy as a Function of the Research, Development and Deployment Status of a Project

When considering single-point estimates one must realize that estimates are made several times over the research development and deployment (RD&D) lifetime of any project (not just in the early R&D stages), be it pioneer or conventional, and the level of detail in each

differs widely. D. H. Allen et al.[17] discuss five types of single-point capital cost estimates for chemical process plants. These are the types of estimates often referred to in the literature of the American Association of Cost Engineers (AACE) and which are most often used for conventional technologies.

The first, the "order-of-magnitude" estimate, can be arrived at by the ratioing of previous similar cost information on particular process attributes if such information exists. For most processes in the early R&D stages, however, previous data may not be available and an "order-of-magnitude" estimate may be the result of very basic process science and design calculations coupled with rough capital cost estimates for the major process equipment items. A multiplier is often used to cover balance-of-plant items. In such cases the first estimate becomes a "back of the envelope" type estimate, and may incorporate significant developer optimism. (Optimistic productivity and production cost projections are often injected into such order-of-magnitude estimates to justify continued R&D expenditures from project funding sources.)

The second or "study" type estimate represents the first significant use of data developed by scientists, engineers, and designers and incorporates knowledge of the material and energy flows along with layout and specification of major equipment, including some balance-of-plant items. In a large-scale, first-of-a-kind project, the R&D program at this stage may be at the point where process productivity is still the dominant uncertainty. This "study" type estimate may still include

significant developer optimism in both equipment cost and productivity projections.

The third, the "conceptual" or "initial budget," estimate is usually made when the decision to embark on a large-scale project is imminent. Sufficient data are made available for budget preparation. At this point, time-phased data such as a construction timetable and capital spending pattern are incorporated into the estimate. All known balance-of-plant and process-support items are included. The productivity of the process has usually been demonstrated at a scale, such as in a pilot plant, supporting the productivity projection upon which this estimate is based.

The fourth or "project control" estimate is highly definitive and includes detailed engineering data and the most important process equipment drawings. At this point the decision to proceed with the project has been made and a significant amount of cost data from equipment suppliers is available. Architect-engineering firms are often brought into the project for preparation of this level of estimate.

The fifth or "firm" estimate consists of contractors' estimates and complete engineering drawings and specifications. It is frequently updated during the course of the project, often by use of a computerized project management system.

Allen's article[18] gives error ranges for these five classes of capital cost estimates for conventional chemical plant projects for which process performance was not an issue: (1) "order of magnitude" estimate, greater than ±30%; (2) "study" estimate, ±30%; (3) "initial budget" estimate, ±20%; (4) "project control" estimate, ±10%; and

(5) "firm" estimate, ±5%. The range of +60,-90% discussed by Nichols[19] for the class closest to (2) above indicates that perhaps early estimates are even more inaccurate than stated by Allen.[20] Since new technology projects involve nonconventional equipment and performance uncertainties, the error ranges on such estimates may be even larger than those cited above for classes (1) or (2).

The data in the Rand study,[21] which uses a numerically different but structurally similar rating system for classes of estimates, confirm this observation by showing that the average pioneer plant capital cost estimate for a similar class of early estimates was low by 52%, with best and worst estimates being low by 28% and 74%, respectively. Figure 3.1 shows a composite plot of the Rand estimate ratio data compared with similar data from Nichols[22] and Allen.[23]

General Observations on Unit Cost Trends

It is of interest to plot ratios of this type on a process development time-line, in this case with unit production costs rather than capital costs, and note the S-curve shape of a time plot of the ratio of the nth unit cost estimate to the first unit cost estimate, where the Nth estimate in this case can be considered to approximate the experienced unit cost. The use of unit costs has the advantage of folding in productivity (performance) as well as total annualized production costs. As in earlier discussions, the effects of inflation are removed.

A plot typical of pioneer process development projections is shown in Figure 3.2. The left part of the curve represents early economic .

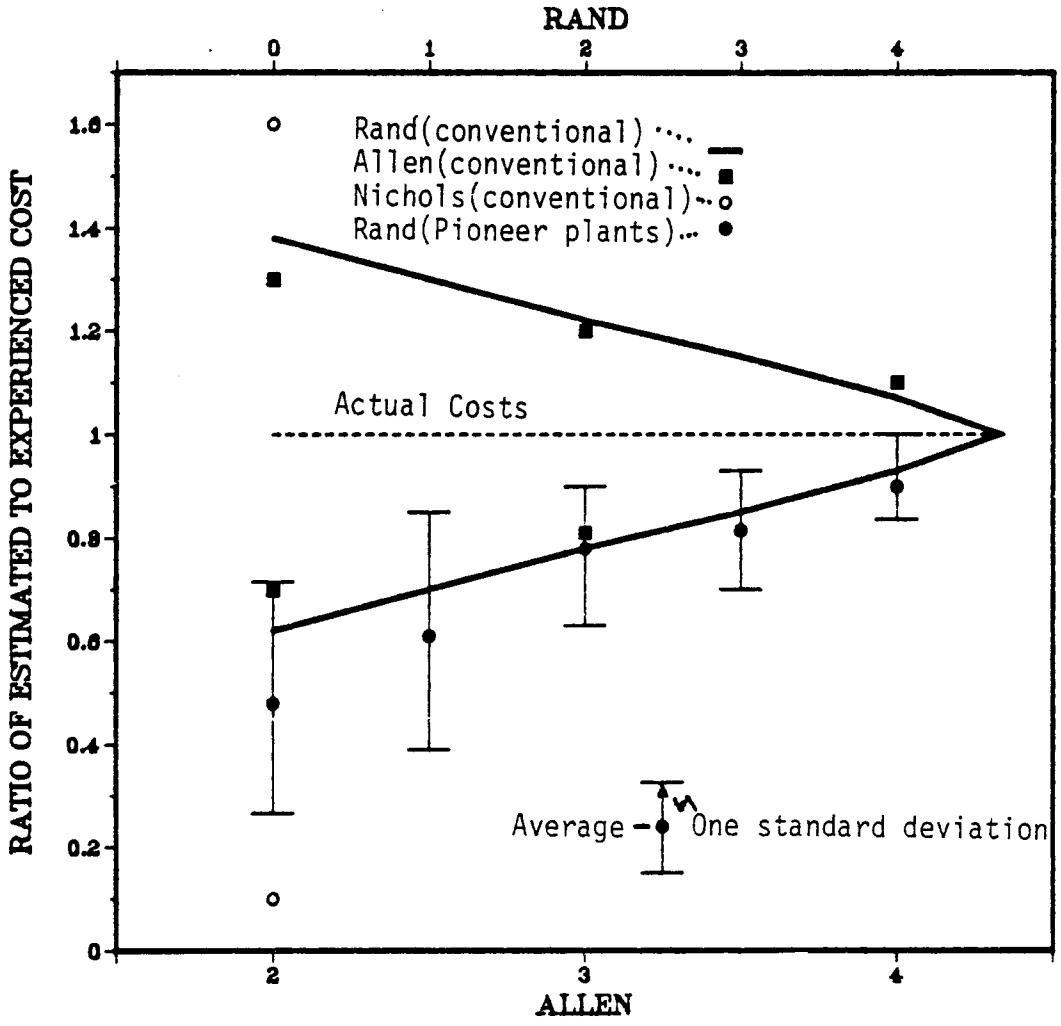


Figure 3.1

Ratio of Estimated to Experienced Costs as a Function of Estimate Class for Conventional and Pioneer Chemical Plants

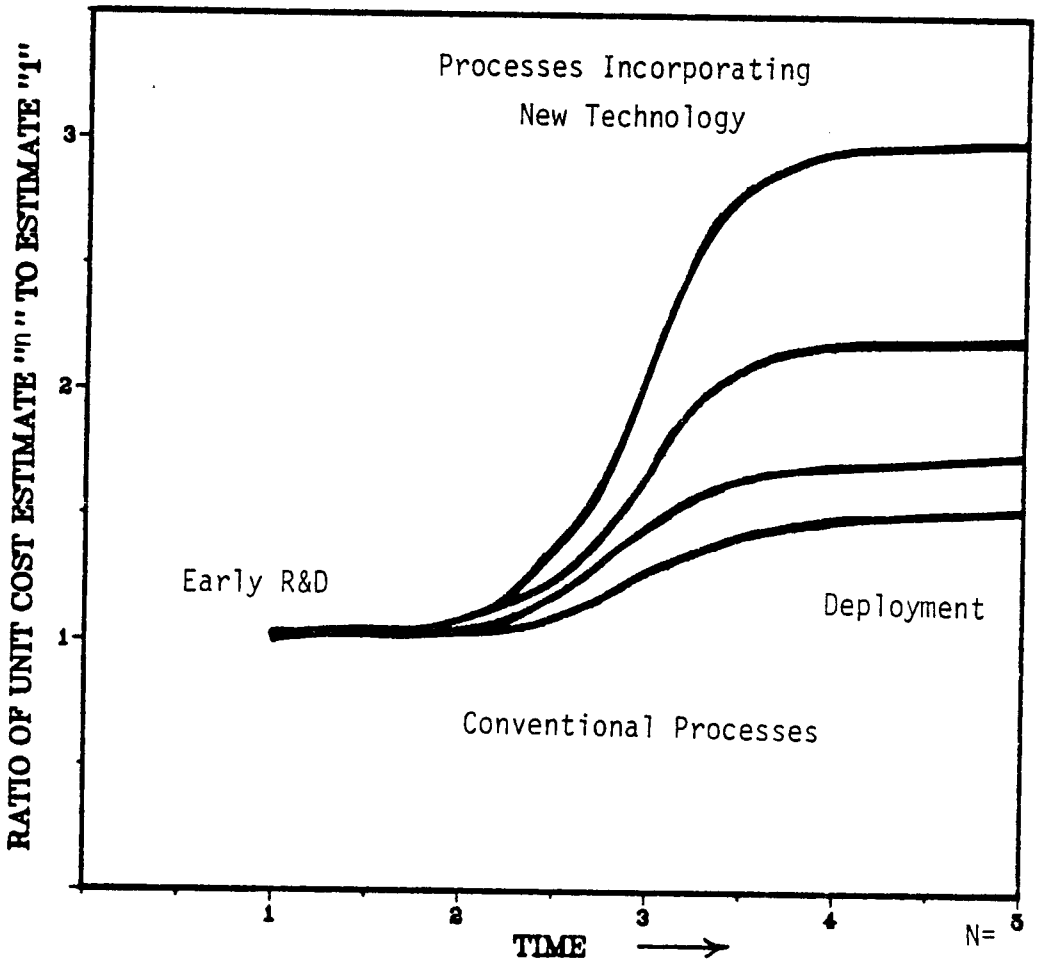


Figure 3.2

Family of S-Curves Depicting Increase
of Estimated Unit Cost with Time

analyses, which usually include a significant degree of developer optimism. Beneath the inflection point are the first preconceptual plant designs and above this point are later, more detailed, designs for proposed facilities. For a pioneer process, it is difficult to separate the unit cost components of this curve attributable to underestimated production costs and overestimated productivity. Experience has been that the unit cost ratio could follow a similar shaped S-curve even if process productivity were predicted exactly. The effect of poorer-than-originally-expected process productivity manifesting itself in the later development stages tends to steepen this curve. If unit cost ratio experiences for pioneer processes under development are included along with unit cost ratio experiences for conventional processes, a family of S-shaped curves results, with the conventional technology curves bounding the lower end of the region. The upper region poses a significant problem for the decision-maker or strategic planner, since essentially it indicates that early unit cost estimates for first-of-a-kind processes are merely optimistic educated guesses. For this reason, economic projections for such technologies often lack credibility, especially outside the R&D community.

Attempts to Understand Capital Cost Misestimation for Conventional Chemical Processes

The effects of tangible or identifiable factors on annual production costs, of which the latter includes both recovered capital and annual operating costs, can be handled by well-documented techniques such as sensitivity analysis. Relatively little appears in the open

literature, however, on determination of less tangible cost-driving factors; i.e., those, such as process complexity or project management ability, which are not definitive or easily quantifiable, but definitely have cost effects. What does exist in the literature deals primarily with conventional chemical processes in the later stages of cost estimation. In essentially all the literature reviewed, capital costs were considered, with operating cost considerations omitted.

J. W. Hackney[24] deals with the subject of these less definitive process attributes in detail and proposes use of an Uncertainty Rating Summary Form in conjunction with a cost estimating task. A weighting system tied in with use of a rating point system is applied to various research, development, and engineering data available for the project. From this procedure an estimating error is projected. The five main headings in the list of data are (1) general project basis, (2) process design, (3) site information, (4) engineering design, and (5) detail design. The qualitative factors affecting capital estimate accuracy are discussed in detail and fall into the five following basic categories: degree of project definition, accuracy of forecasting job conditions, the estimating method used, the adaptability and accuracy of available cost records, and the skill of the estimator. Essentially a five by five evaluation matrix is constructed and a composite score calculated.

The data base for Hackney's study constitutes conventional processes where performance is not important, hence his method has very limited utility for first-of-a-kind process technology.

The Rand Pioneer Plant Study's Attempt to Understand and Correct Capital Cost Misestimation

The first section of the Rand document[25] discussed the problem of underestimation of capital costs in pioneer chemical process projects; however, the second section suggested a methodology for quantifying the two components which contribute most to misestimation of unit production costs, i.e., failure to achieve desired performance and unanticipated capital cost growth, exclusive of inflation. For their data base the Rand study considered one class of pioneer technologies, namely, plants involving liquid or solids processing, which at the time of the predictive estimate were at an R&D stage far enough along to be more than first-of-a-kind processes but did not constitute the label of completely conventional. In order to quality as "pioneer," the process had to incorporate at least one commercially unproven major step.

The Rand study authors followed 44 such projects from the earliest estimates of cost and productivity through to their completion or abandonment. Accordingly, Rand had available for their analyses, series of interim evaluations as well as actual or experienced cost and operational data for the projects they studied. Qualitative attributes of each process, such as process complexity and "newness" of process steps, were studied; and in order to arrive at a quantitative representation for each attribute, a numerical scaling system was devised to assign values to the attributes common to all 44 processes. It was necessary for Rand to structure the processes in terms of such defined, but very arbitrary, qualitative attributes.

A regression analysis was performed to determine the effect of the numeric representation of these attributes on the estimated-to-actual capital cost ratio. The attributes with the highest correlation were fitted by the Rand authors to algebraic relationships as shown below.

Cost growth experience. The following expression was derived by the authors of the Rand study to quantify the cost growth phenomenon:

$$\text{COST GROWTH FACTOR (CGF)} = \left(\frac{\text{Estimated Cost}}{\text{Experienced Cost}}\right)$$

$$= 1.12 - 0.00297\,(\text{PCTNEW}) - 0.02125\,(\text{IMPURITIES})$$
$$- 0.01137\,(\text{COMPLEXITY}) + 0.00111\,(\text{INCLUSIVENESS})$$
$$+ \text{LRD}\,(\text{PROJECT DEFN})$$

Possible Cost Growth Values: CGF $\geq$ 0

[CGF < 1.0 if cost growth occurs]

where:

PCTNEW = % of capital estimate incorporating technology unproven in commercial use

Value Range: 0 to 100

IMPURITIES = Assessment by industry engineers of difficulties with process impurities encountered during development

Value Range: 0 to 5

COMPLEXITY = Block count of all major process steps in plant

Value Range: 1+

INCLUSIVENESS = % of actual required major process equipment items (including balance-of-plant items) included in estimate

Value Range: 0 to 100

PROJECT DEFINITION = Level of site-specific information and engineering included in estimate

Value Range: 2 to 8

LRD = Coefficient for variable PROJECT DEFINITION

= -0.04 if process has been proven on pre-commercial or commercial scale

= -0.0636 if process is in R&D stages

A mean value of 0.78 was obtained by Rand for the composite COST GROWTH FACTOR for the 44 process plants comprising their data base. This is the same as saying that an average plant estimated at $100 million actually experienced an inflation-free cost of (1/0.78) x 100 $MM or $128 million.

Plant performance shortfalls. The following expression was derived by the authors of the Rand study to quantify the productivity degradation experience:

PERFORMANCE DISCOUNT FACTOR (PDF) = Actual average production 7 to 12 months after start-up as a percent of plant design capacity production

Value Range: 0 to 100+

= 85.77 - 9.69 (NEWSTEPS) + 0.33 (BALEQS) - 17.91 (SOLIDS) - 4.12 (WASTE)

where:

NEWSTEPS = Number of process units incorporating technology unproven in commercial use

Value Range: 0 to Total No. of Blocks

BALEQS = % of heat and material balance equations based on actual data from prior plants

Value Range: 0 to 100

WASTE = Assessment by industry process engineers of difficulties with waste handling encountered during development

Value Range: 0 to 5

SOLIDS = Designation that a plant processes primarily solid feedstocks or products

Value Range: 1 if Solids

0 if No Solids

For the 44 process plants in the Rand study, the mean PERFORMANCE DISCOUNT FACTOR was 72%.

Critique of Rand Methodology

The above two factors, cost growth (CGF) and performance discount (PDF), represent adjustments which can be applied to productivity and capital cost estimates on pioneer chemical process plants. A difficulty with the Rand factors is that they are not both simultaneously and uniformly applicable to estimates made at any time during the RD&D life of a project. The PDF, for example, only compares the achieved production of a plant 7 to 12 months after start-up with the design production. No claim was made that the PDF could be used early in the development

program to predict performance shortfalls to be experienced in the future production operations.

The Cost Growth Factor, as described by the Rand report, appears to be most applicable over the latter stages of the RD&D life of a project. This observation is based on the fact that Rand's data base included projects that had at least some pilot plant experience and for which hardware requirements were well known. If the Cost Growth Factor were extended to projects in the early RD&D stages, its value would be expected to deviate even further from unity than the factors derived for the Rand processes. The Cost Growth Factor (CGF) is in large part a measure of the level of design detail available in a given capital cost estimate, hence, it should approach 1.0 for higher classes of estimates. The CGF does not include annual operating costs, which in addition to annual productivity and capital costs, are important components of the total unit product cost. If the CGF, as defined by Rand, is to be used to adjust an estimate, its reciprocal is multiplied by the estimated capital cost. The cost growth factor is more general (i.e., less specific to the type of generic process studied) than the performance discount factor; hence, the nature of its constituent parameters suggests possible attributes which can be used to predict the costs of other classes of processes, even those in early R&D stages and utilizing first-of-a-kind technology.

In critiquing the Rand Pioneer Plants Study, one must consider that most of their data base consisted of processes in later development stages than those to be considered by the methodology presented in this dissertation. This suggests that predictive use of the Rand algorithm

for cost growth and performance degradation may be very hazardous for new processes in early R&D stages.

The fact that all of the processes in the Rand study utilized conventional chemical engineering operations also implies that it would be presumptuous to extend these algorithms to technologies which do not use such unit operations. In the User's Manual[26] for the Rand study this warning is implied, for it is suggested that the algorithms not be utilized for electric power plants, solar technologies, pipelines, or storage facilities. It was stipulated that plants to be evaluated should possess linked steps forming a continuous process. Some of the quantitative attributes needed to calculate the Rand cost growth factors and performance discount factors were based on a criterion applied to the block count of process steps. Two of these criteria included "newness" and "complexity."

The idea of breaking a chemical process down into steps or process modules and estimating the cost therefrom is not a new one. Authors such as De Cicco,[27] and Zevnick and Buchanan,[28] and Klumpar, Fromme, and Brown[29] suggest that crude capital cost estimates for chemical processes can be derived quickly by utilizing the block count of process modules as a major variable in a total capital cost computation algorithm. These techniques, along with the Rand approach, do not appear to be applicable to many energy-related processes such as power plants and uranium enrichment plants where a large percentage of the capital cost can be attributed to one or two expensive classes of hardware. As an example, most of the cost of a nuclear reactor is dedicated to the pressure vessel and its constituent core and control mechanisms.

Other equipment, such as the electrical generators and the condenser, bear small costs in comparison. Similarly, in a gas centrifuge enrichment plant such as GCEP, over 40% of the capital cost is dedicated to the purchase of centrifuge machines. Other material handling steps in the process are also small in comparison.

For the processes which this dissertation considers, it is the innovative step itself which should constitute the attention of the evaluator. The major uncertainties are still associated with the new technology rather than the configuration of the overall process. For this reason correction factors of the type suggested by the Pioneer Plants Study[30] have very limited usefulness and can even mislead the evaluator.

If one starts with the realization that the Rand work has identified areas which historically have proved to be stumbling blocks to good cost projections, and then works hard to tighten the estimating procedure in these areas, one should not need or desire to apply Rand's correction factors to the results obtained.

The Incorporation of Uncertainty

The key to resolution of the production cost underestimation and productivity overestimation problems lies in the construction of a credible process assessment model and construction of a method for handling process uncertainties. Model building is process-specific, hence a literature review covering modeling techniques would be pointless. Statisticians and operations research investigators, however, have developed many generalized approaches for uncertainty

analysis, and the most important techniques along with some relevant applications are discussed below.

Analytical Methods for Propagation of Uncertainty

S. W. Hess and H. A. Quigley[31] summarize several methods for determining venture profitability uncertainty in the chemical process industries, but they consider financial rather than technological factors. Some of these suggested methods are analytical, i.e., they do not involve statistical sampling techniques.

One of the simplest analytical techniques considered in their review is that of sensitivity analysis. This is normally accomplished by tabulating values of the output figure of merit, in their case a profitability index such as rate of return for different values of the key input variables, which are usually submitted one at a time to the model. This single value sensitivity study (SVSS) technique is useful in identifying the input variables having the most influence on the output and for identification of significant trends; however, a major weakness is that it cannot determine the likelihood or probability of obtaining any particular value of the figure of merit.

Another analytic method of uncertainty propagation is proposed by W. L. Gore[32] and R. H. Carter[33] in separate articles. The problem is simple for cases where input normal probability density functions (pdf's), which are most often referred to as "distributions," are known, and for which the return function R=R (A, B, C, ...), with maximum and minimum limits on the inputs ±a, ±b, ±c, etc., can be algebraically represented. The maximum and minimum limits on R, i.e., ±r, can then be

approximated analytically as:

$$+r = [(\frac{\partial R}{\partial A})^2 \ (a)^2 + (\frac{\partial R}{\partial B})^2 \ (b)^2 + (\frac{\partial R}{\partial C})^2 \ (c)^2 + \ldots \ ]^{1/2}$$

$$-r = [(\frac{\partial R}{\partial A})^2 \ (-a)^2 + (\frac{\partial R}{\partial B})^2 \ (-b)^2 + (\frac{\partial R}{\partial C})^2 \ (-c)^2 + \ldots \ ]^{1/2}$$

by derivation from a Taylor series expansion. The limits ±a, ±b, etc., represent a given number of standard deviations, $n\sigma$. from the mean. Such an analytical method for what is also called "propagation of variance" or "propagation of error," depends on random variables A, B, C, etc., being normally distributed and statistically independent, and the confidence intervals or number of standard deviations from the mean for ±a, ±b, ±c, etc., being the same. This technique, which is useful in estimating upper and lower $n\sigma$ values (or is the standard deviation) on R, does not calculate its probability density function (pdf). The limitations on this analytical method are so severe as to preclude its use in analysis of complex systems.

These Taylor series expansion methods can be used successfully in certain types of linear models to quantify output parameter uncertainties as a function of input data uncertainties. R. W. Peelle et al.[34] use such an analytic method to develop an uncertainty matrix (variance-covariance matrix) for the important parameters of their long-term Energy Analysis Package which they manage for the Department of Energy.

The problem of calculating the probability density function for a continuous function R=R (A, B, C, ...) can be approached analytically

for simple functions, such as products, quotients, and sums, of normally distributed independent variables A, B, C, etc. If these variables are not independent, the resulting expressions are complicated by covariance terms. The equations for functions of means and variances of normal distributions are treated in many texts[35],[36] and papers[37],[38] and are frequently used in quality control applications such as the calculation of dimensional tolerances.

The problem is that hard-core analytic models based on theorems of mathematical statistics are so limited by the requirements for tractability of solution that they cannot reflect the complexities of real problems.

Non-Analytic Methods for Propagation of Uncertainty

The real breakthrough in dealing with uncertainty associated with complex functional relationships was the development of the Monte Carlo or simulation technique and its application by D. B. Hertz[39],[40],[41] for use in analysis of uncertainty in financial and marketing environments.

When such "investment risk" analysis is utilized in the conventional fashion, there usually exist significant data bases in areas such as sales, price, and cost history, and marketing demand data from which uncertainty inputs can be bounded. The science and engineering--hence the productivity--of the particular production enterprise are usually not an issue. This Hertz application of the Monte Carlo technique coupled with appropriate models, and more commonly referred to as simulation, is typically used to assist the decision maker in choosing, from

a field of alternative venture scenarios, the venture which is most likely to yield a high rate of return or net present worth.

The user of this risk analysis method must develop a set of probability density functions (pdf's), more commonly referred to as "distributions," for the input variables of interest. These pdf's can sometimes be derived or extrapolated from experimental and historical data; however, often more heuristic methods of derivation are necessary. Given pdf's for key inputs, a digital computer can be used to select randomly an ensemble of input values for use in the system model. The system model is run with this ensemble of inputs to generate one or more figures of merit for the process. By repeating the calculation many times, probability density functions for the figures of merit are also obtained. The Monte Carlo simulation method of multivariable sensitivity studies (MVSS) is the only usable analysis technique cases where complex models are involved. Figure 3.3 from Hertz's original paper[42] illustrates the steps in this procedure along with some typical inputs.

The literature contains many examples of the application of Hertz's Monte Carlo simulation in financial analysis of process industries. These are mentioned merely to show that the method enjoys widespread acceptance in the field of venture analysis. A dissertation[43] by Jennings outlines the development and use of a sophisticated FORTRAN computer program (GENECON) for generalized financial risk analysis for use in the chemical and petrochemical industry. D. Allen[44] discusses the use of the Monte Carlo method in discounted cash flow analysis. A. K. Sunol[45] has developed an Advanced Chemical Process Economics

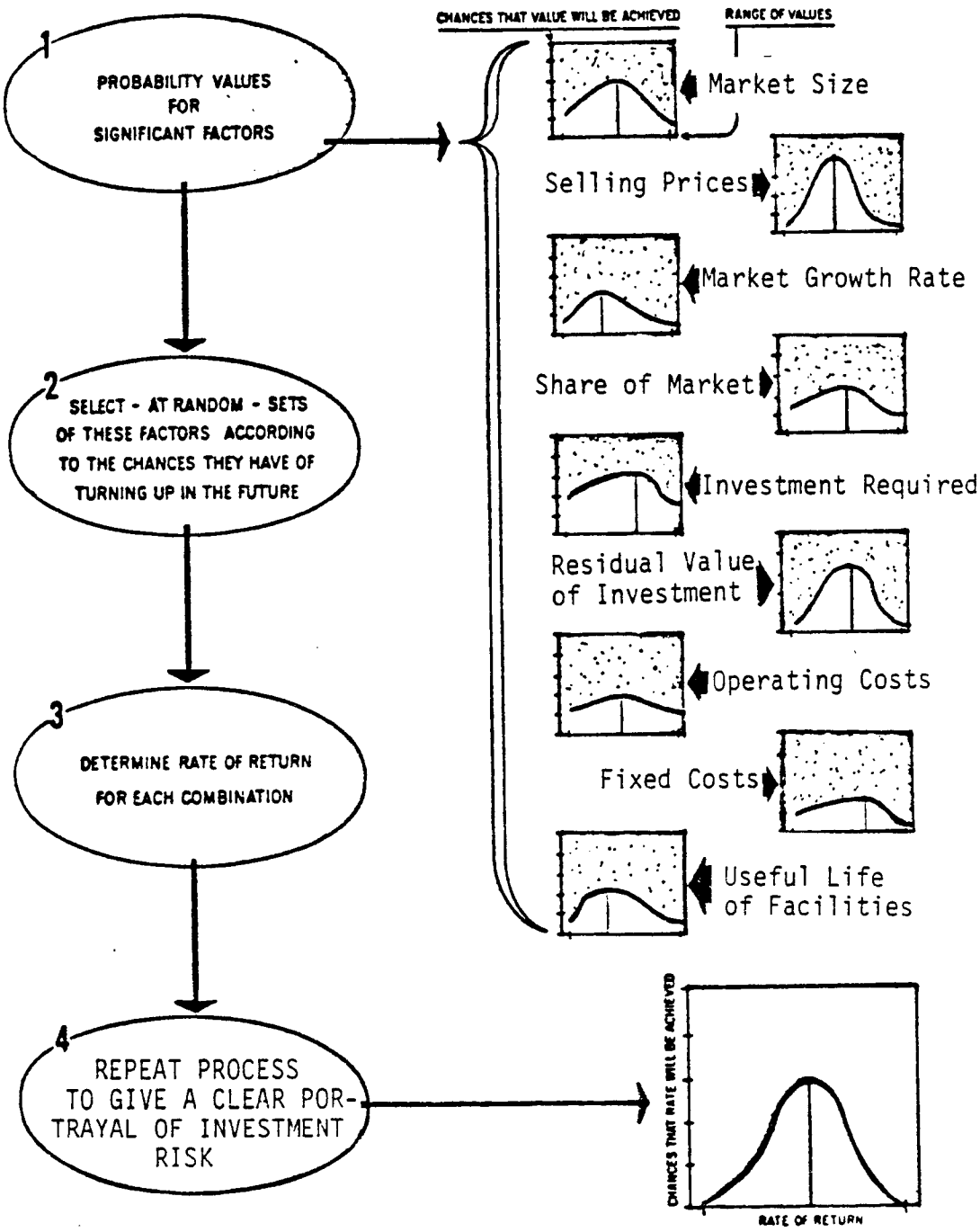


Figure 3.3

The Hertz Application of the Monte Carlo Technique: Simulation for Investment Planning

Source: Hertz, D. B.,"Risk Analysis in Capital Investment," Harvard Business Review, Jan.-Feb. 1964.

computer simulation code (ACPE) which is used for venture feasibility studies on coal conversion projects. W. G. Sullivan and R. G. Orr[46] present a short simulation code for use in simple engineering economy problems dealing with net present worth.

The simulation method has been applied in the area of venture analysis for many years. The difficulties in applying it to economic evaluation of process technology in the early R&D stages are the following:

1. Often little historical data, such as that available for conventional process venture decisions, are available. The process assesser, therefore, must rely on more difficult-to-obtain experimental or theoretical data. Measured values and ranges for first-of-a-kind process parameters are often not available and educated guesses must be used. More importantly, when the "best guess" for a variable value is hard to come by, the range (width) of the variable's distribution is even more difficult to obtain. Bounding the input variable ranges requires considerable analysis and a thorough understanding of process issues.

2. When describing physical and chemical systems, as well as purely economic ones, there may exist unknown significant interdependencies between productivity-determining input variables. The process productivity model may not describe all phenomena and interdependencies present in a process and the model is often based on theoretical calculations not yet verified by experiment.

3. In a process model, one has the opportunity to re-optimize the design for any given set of process inputs. If these opportunities are not recognized and included in the performance and design model, the

Monte Carlo procedure for selecting inputs may generate cases which are physically unrealistic.

All of these problems will be treated to some degree in Chapters V and VI and solutions proposed. In doing so it will be shown that the Monte Carlo method represents a powerful tool for evaluating complex technologies.

The Need for Technological Forecasting

Lack of an historical data base for immature or new projects necessitates provision of other sources of information both for input pdf's for Monte Carlo simulation. In most cases one must rely on theoretical projections, if available, or extrapolation of historical data from other R&D programs. Some guidance in this area can be obtained from the relatively new science of technological forecasting. Martino[47] defines a technological forecast as a prediction of the future characteristics of a useful machine. The word "machine" is interpreted in the broad sense to include tools, techniques, and procedures; and characteristics refer to the physical description and performance of the machine. An example of a technology forecast might be the projected energy output of a particular class of laser to be deployed ten years in the future or the projected mileage for future automobile tires.[48]

The decisionmaker's assessment must be examined and challenged by experts, and procedures for effectively arriving at some sort of consensus have been devised. A procedure known as Delphi,[49] originally developed by researchers at the Rand Corporation, allows the formation

of a group opinion. Deliberation takes place in several rounds or iterations until a statistically significant majority viewpoint on a particular issue prevails. As a means of reducing personal and institutional bias, the identities of the group members are not made known to each other.

Another procedure for technology forecasting and also for uncertainty input determination is that of peer review, which is a less formal means of collective judgment. Peers constitute experts or developers working in the same technology areas. By review is meant the free exchange, discussion, and criticism of experimental and theoretical data related to the technology of interest. Peer review has an analog in the use of referees to evaluate the merit of articles submitted to learned journals.

When this evaluation methodology was used by the Department of Energy[50] and its contractors for selection of an advanced uranium enrichment process, peer review played a vital role in identifying issues and evaluating the quantitative technical inputs required.

Interpretation and Use of Evaluation Results in Overall Process Assessment

Once an effective means of assessing economic potential is in place, one must consider its applications. The method can be used to decide whether to continue development or even to deploy a single technology under investigation. One of the most frequently discussed applications is that of selecting a candidate for further development among alternative processes undergoing R&D. The selection procedure should consider comparisons between the Monte Carlo-generated output

distributions obtained for the same figures of merit for each process. In making such comparisons, one must include somewhat subjective characteristics, such as the evaluator's attitude toward risk. The process of quantifying attitude toward risk is known as utility theory. Techniques are available for assessing the probability data in conformity with an evaluator's attitude toward risk-ventures and these are the subject of papers by Holland et al.[51] and Thorne[52]. The type of question which must be considered in utility theory is that of how much financial risk is acceptable. In this study the problem of quantifying attitudes toward risk is not considered. It is more important that the evaluator at this point understand the technology itself and the statistical methodology behind the uncertainty evaluation.

Literature Review Summary

It has been shown that the literature documents in some detail the inaccuracy of performance and cost estimates for both conventional technologies and technologies especially in the late RD&D phases. The Rand "Pioneer Plants" study was an attempt to document and correct estimating inaccuracies; however, it is applicable for a very limited class of processes.

The Monte Carlo simulation method represents a major advance in analysis of uncertainty; however, its use in economics has been confined mainly to financial and marketing analysis of conventional manufacturing enterprises.

For analysis of the technological uncertainties associated with new uranium enrichment techniques, the Monte Carlo method was extended for

use with process performance, design, and cost models. It was so successful when used in this context, that it became quickly apparent that the method could be extended to nearly any process technology possessing uncertainties in science or engineering. For this reason, the method warranted publication.

The following chapters do not consider a particular detailed application, rather the general method is discussed; i.e., when to use it, how to use it, what it can and cannot do, and how to interpret its results. An illustrative detailed example technology is examined in Appendices I through K.

CHAPTER IV

APPLICABILITY OF METHODOLOGY

The Two Major Criteria

Applicability of this methodology requires an examination by the potential user of (1) the description or nature of the technology, and (2) the nature of the modeling task as related to the uncertainties and figures of merit of interest. The first of these is important, since the methodology was developed for use with special classes of technologies and is not meant to be applied to all projects, especially those for which conventional economic assessment techniques would suffice. Certainly there are individual elements of this methodology which can be applied to more general process applications; however, the intent is to here present the reader with a comprehensive methodology for specialized uses and to, beforehand, indicate to him or her its most appropriate application.

The second criterion, the nature of the modeling tasks, asks which of three tasks, development planning, process assessment, or strategic planning, is the user most interested in addressing. It also asks whether the task is appropriate to the nature of the uncertainties. As mentioned in Chapter I the bulk of this methodology is appropriate only for the second task, i.e., process assessment in which technological uncertainties are examined.

Figure 4.1 is a stepwise further breakdown of the two criteria the user's application must satisfy. Each step is considered in more detail in the following sections.

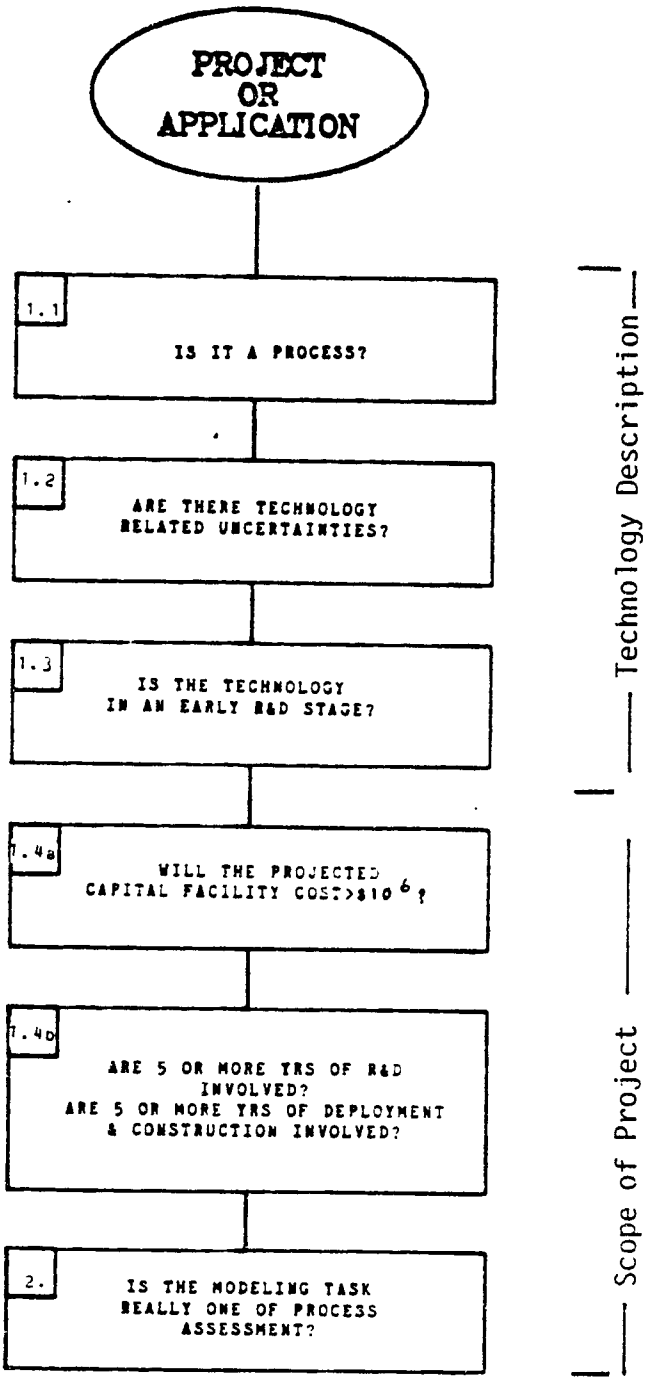


Figure 4.1

Applicability Criteria for the
Economic Evaluation Methodology

Nature of the Technology

In determining whether the proposed project or application is suitable for the method, four questions are asked of the potential user:

1.1 Does the proposed project represent embodiment of a process?

1.2 Is the project based on application of a new discovery or innovation for which uncertainties in the technology exist that might reduce its economic potential?

1.3 Is the project in the early RD&D stages?

1.4 Is the scope of the project sufficiently large that it warrants the effort required for successful use of this methodology?

Each of these questions will be discussed separately and the reader will be given guidelines for use in making proper judgments.

Morphology of a Technology: Is the Proposed Project Really a Process?

A functional hierarchy, in the form of a decision tree, can be used to classify a project in the same way a biologist classifies an organism into phyla, classes, orders, families, etc. The morphological criteria for each branch will not be as clear-cut as for organisms; however, the analogy is still an instructive one. Figure 4.2 illustrates the generic classification of projects in network form. A description of each level and its attributes will be given along with technology examples. Differentiation can be made mainly on the basis of how performance is defined and how capital and operating costs are distributed over the life cycle of a project.

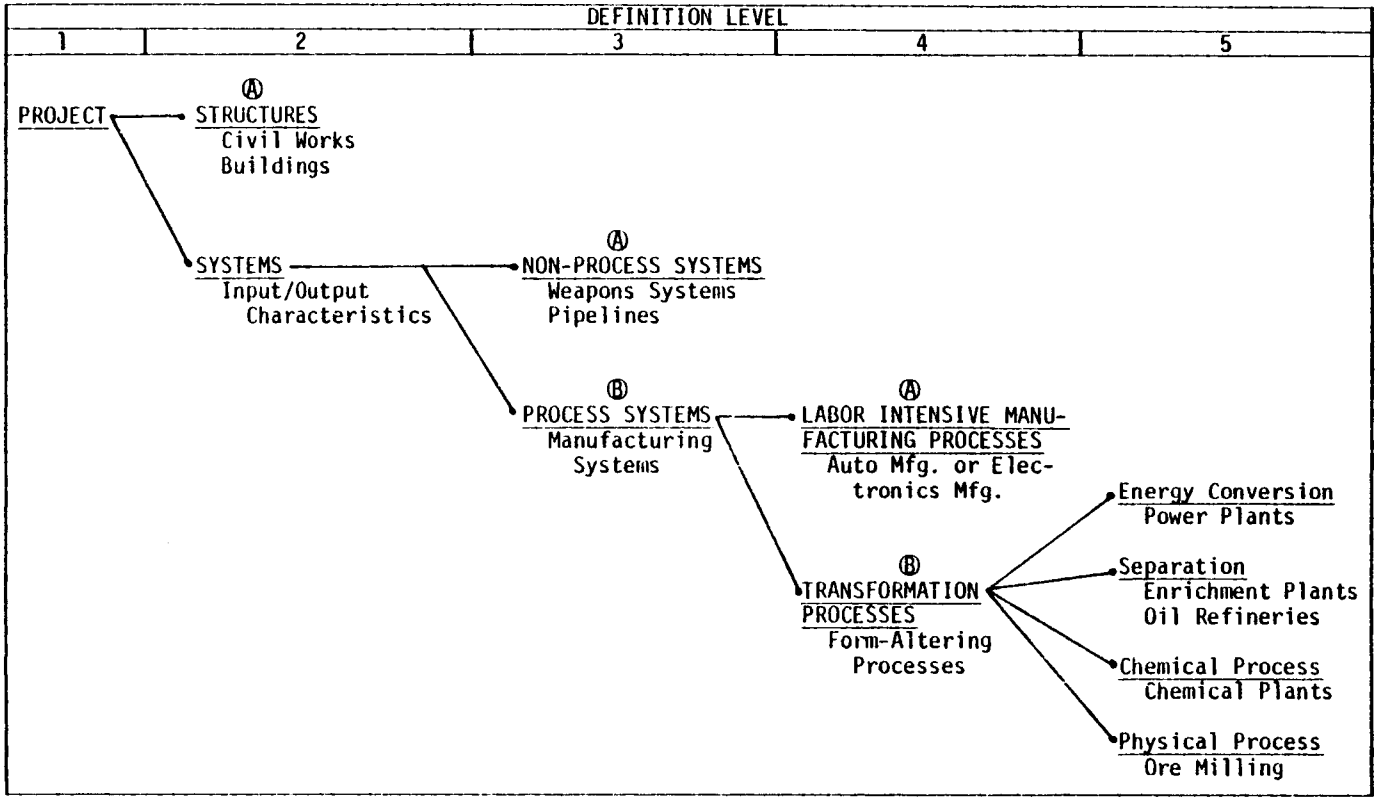


Figure 4.2

Project Morphology

Level 1. The Project

A project is here defined as the large-scale embodiment or application of a particular technology. It represents the goal toward which the RD&D, engineering, estimating, and construction efforts are oriented.

The project costing life cycle for this methodology will exclude the R&D portion of the total RD&D effort and is assumed to begin when a decision to deploy a technology on a large scale is made. The front-end project costs consist of engineering and construction activities; and the remaining costs constitute the annual operating costs, which normally span the largest fraction of the total duration of the project life cycle and represent the costs of maintaining and operating the facility. Decommissioning, destruction, or shutdown costs are incurred at the end of the life cycle. In the hierarchy presented, two types of projects are discussed--structures and systems.

Level 2-A. Structures

A structure represents a large-scale project for which performance is not measured in terms of an output and for which the annual operating costs are in general a small fraction of the construction cost. The best examples are civil works such as bridges and buildings. The success of a structure is determined by the availability of the structure for use and, to a lesser degree, the percentage of time that it is actually being utilized at full capacity. A bridge, for example, is designed to be available to the user at nearly all times; however, the

planners and designers usually recognize that it will only operate at its full traffic capacity for a few hours a day.

Most structures utilize conventional civil engineering technology where rated performance is represented by the design capacity, and uncertainty in the engineering calculations is largely eliminated by the use of appropriate building codes. Safety of a structure is supposed to be guaranteed by following the appropriate codes and standards in the design work. Construction or capital cost estimation, however, is of paramount importance, and uncertainties are present in materials and labor costs. Since interest charges accrue during construction, project timing is an important consideration. Factors such as strikes, weather, and material shortages can impact construction timing considerably. The particular methodology here presented is not appropriate to the analysis of structures.

Level 2-B. Systems

A system differs from a structure in that it displays dynamic behavior, i.e., it can be represented as a transfer function which when acted upon by an external influence or forcing function elicits a dynamic response. Controllability and high availability are important performance criteria. As with structures, the percentage of time a system is actually in use or operating at rated capacity may be a secondary determinant of its success. Typical examples include production processes, transportation systems, weapons systems, and computers. When compared to structures for which construction costs predominate, systems are likely to have an increasing fraction of their life cycle costs dedicated to operating and maintenance.

Systems are more amenable to modeling efforts since desired system performance and the factors which affect it are important determinants of its cost. Modeling of system performance is sometimes referred to as input/output modeling. The category of systems will now be broken down into non-process systems and process systems for further discussion.

Level 3-A. Non-process Systems

Most non-process systems spend a significant portion of their life cycle in an idle or inactive mode; however, their reliability must be such that they will perform perfectly whenever called upon to do so. Weapons systems and safety systems constitute good examples. As an example, a laser-based defense against incoming missiles, would have to exist in a mode where it could be activated at any instant and exhibit 99.99%+ effectiveness, e.g., high reliability. The laser systems involved, however, will be in an inactive mode during 99%+ of their lifetime. The same could be said for the emergency core cooling system (ECCS) in a nuclear power reactor. For non-process systems, reliability and capital cost are the predominant figures of merit and are themselves related. Cost effectiveness is a frequently used term which represents a figure of merit that includes both of these elements.

Other non-process systems include those which do not alter material forms, such as transportation systems, pipelines, and conveyors.

Level 3-B. Process Systems

Associated with a process system is creation of a tangible product from inputs of labor, energy, and raw materials, i.e., alteration of a form. In order to be economical such systems are usually designed to

operate continuously or in a sequential batch mode at near rated capacity. To minimize the contribution of capital cost to unit product cost, one wishes to maintain a high onstream fraction, i.e., minimize down time. Performance can be quantified on the basis of comparing actual productivity to predicted productivity. For a process system in general, the post-construction, post-start-up operating costs will constitute a larger share of the total life cycle costs than for a non-process system. Figure 4.3 shows this comparison graphically for structures, non-production systems, and processes. These operating costs must now include raw materials, energy, and replacement component costs in addition to maintenance costs. It is this class of system for which this assessment methodology is most useful.

It is now useful to break down the process system category into two more detailed categories--transformation processes and manufacturing processes--since this designation will have some bearing on the second question concerning the applicability of this method.

Level 4-A. Labor-Intensive Manufacturing Processes

Associated with any process and its constituent raw materials are "value added" steps which ultimately result in a product. In a labor-intensive manufacturing process most of the value added results from stepwise operations performed by humans and the individual machines they operate. This stepwise organization of a process is sometimes referred to as the division-of-labor concept. The manufacturing of most finished industrial and consumer goods such as automobiles, electronic equipment, and furniture are good process examples of labor-intensive processes. The cost of labor per unit of output represents a significant percentage

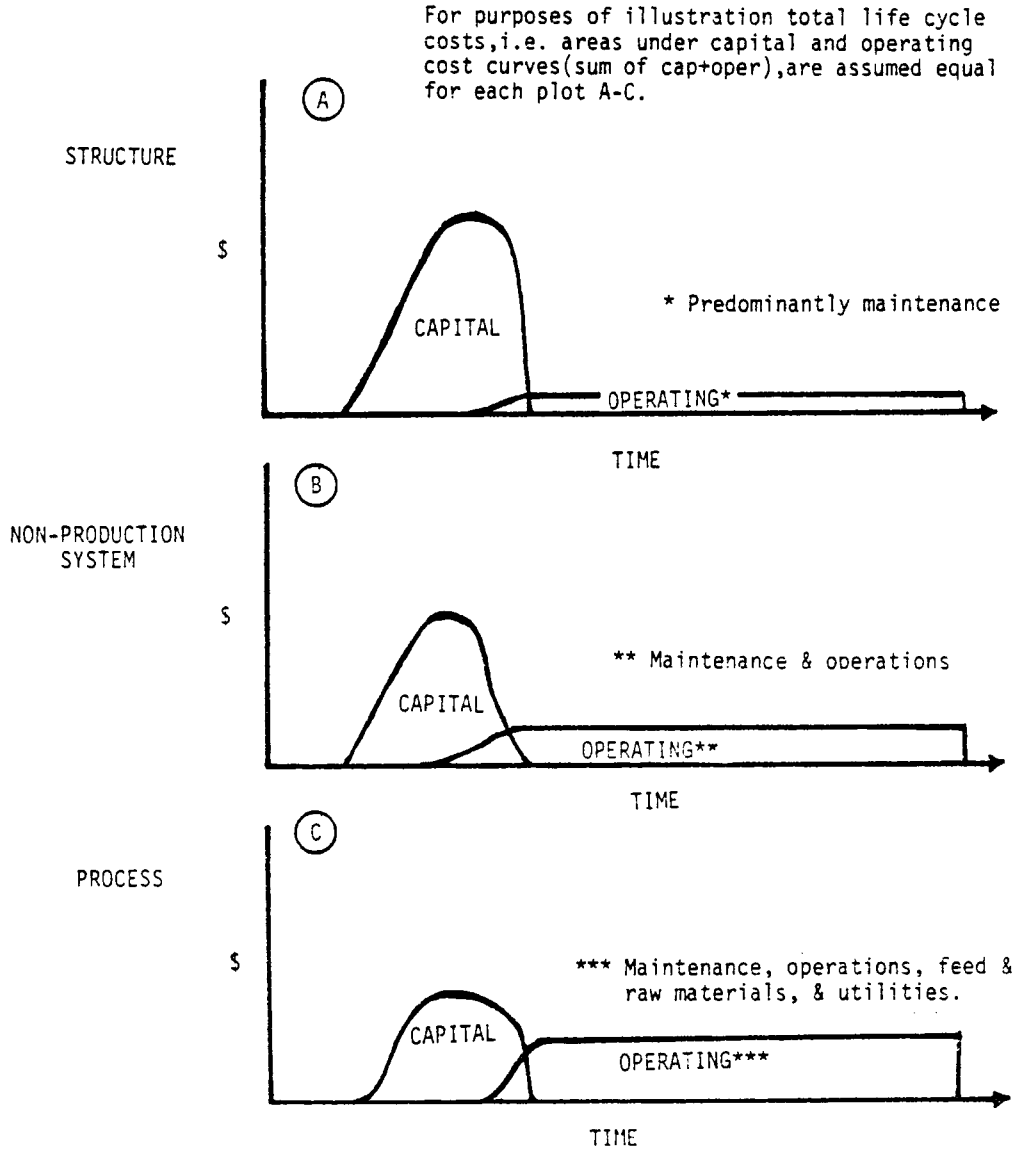


Figure 4.3

Typical Apportionment of Life-Cycle Costs for Differing Project Types

of the operating portion of the unit product cost. Much of the capital portion is dedicated to acquiring tooling and machinery necessary for the manufacturing operations.

A model for a manufacturing process usually contains little process physics and chemistry since most productivity issues are related to labor productivity, quality control, and the reliability of individual machines. Manufacturing processes are usually not modeled so much for purposes of cost estimation as for the purpose of optimization and allocation of human and machine resources.

Level 4-B. Transformation Processes

In a transformation process the value added results from the physical or chemical reconstitution of the raw materials into a useful product. The partially finished materials which represent the inputs to manufacturing processes are in most instances the products of transformation processes. The latter processes are generally less labor-intensive, and the role of labor is more that of a maintenance and operational function. The following represent examples of transformation processes: power plants, chemical plants, uranium enrichment plants, steel mills, ore milling facilities, and oil refineries. The raw material and energy requirements per unit of output, be it energy or a material product, are determined by relationships derivable from the laws of physics and chemistry, i.e., the process science and engineering, represented in each step of the process. The physical operating conditions determine how efficiently the process performs and are themselves constrained by the design limitation of the hardware utilized.

Existence of Technological Uncertainties

Processes which possess inherent technological uncertainties usually are based on a new discovery or unique innovation. In general a proposed application will involve process conditions which were unattainable until development and use of a new invention or innovation. The major uncertainties are often associated with the complexities of transforming a laboratory scale process into a large-scale practical process.

A few examples are illustrative. The possibility of separating isotopes with lasers depended on the invention of the laser, i.e., a device which could produce intense and monochromatic light unlike any conventional light source. Magnetic confinement fusion is made possible by the invention of the superconducting magnet, a device capable of producing the intense magnetic fields necessary for plasma confinement and stability. Large scale application of solar energy for electric power depends on the development of more efficient and less expensive photovoltaic materials.

Recently, innovative process technology has been driven by advancements in four broad areas. These are materials science, electrodynamics, molecular chemistry, and bio-engineering. Table 4.1 shows a few inventions or applications within each technology area.

This assessment method is most applicable to transformation processes involving such applications, since these processes, as opposed to manufacturing processes, are likely to encounter the most difficulty and

Table 4.1

Technology Areas Spawning New
Inventions Applicable to Process Technology

Technology	Process Applications
Materials Science	
High-temperature materials	AVLIS, Fusion
High-stress materials	Gas Centrifuge
Low-corrosion materials	Geothermal Energy
Coatings	Solar Energy
Superconducting materials	Fusion
Semiconducting materials	Computers
Electrodynamics	
Lasers	AVLIS, Fusion
Microwave Generator	Fusion
Photovoltaics	Solar Energy
Plasmas	Fusion
Batteries and Fuel Cells	Power Production
Nucleonics	Nuclear Reactors, Fusion
Molecular Chemistry	
Catalysts	Chemical Synthesis
Metallo-organics	Chemical Synthesis
Polymerization	Chemical Synthesis
Bio-engineering	
Anaerobic Digestion	Pollution Control
Genetic Engineering	Pharmaceutical Production

take the most time in evolving from the laboratory to full-scale production. In nearly every case there is technical innovation and a strong tendency to push physical systems toward operating conditions never before reached.

The uncertainties associated with development of new technologies are usually associated with the performance-related data needed for scale-up and with the cost and reliability of the needed hardware. The model-building and sensitivity analysis methodology described in Chapters IV and V will allow the user to determine exactly where these uncertainties lie. When initially considering applicability, as is the purpose of this chapter, the knowledge that uncertainties exist is often highly intuitive.

Technology Research, Development, and Deployment Status

Along with technology description, research development and deployment (RD&D) status is itself an important criterion in the selection of a modeling technique. The goals and orientation of an economic evaluation effort will be found to vary with technology status and will be discussed below. Five technology RD&D status levels are described below and examples presented. It should be noted that levels beyond just R&D are now being considered, i.e., process deployment. For this reason the acronym RD&D is more appropriate than just R&D. An increasing Roman numeral associated with each RD&D stage has associated with it a decreasing degree of economic and technical uncertainty as the project proceeds toward a reduced-to-practice technology.

RD&D Level I: Theory Development/Scientific Feasibility

Important scientific discoveries often point toward immediately appealing applications which might revolutionalize an entire industry. Once the theory behind the discovery is outlined, one can conceptualize potential applications and begin to calculate the process performance and potential costs. The engineering feasibility of the proposed application may not have even been demonstrated and the only data supporting success of a project might be theoretical calculations and a demonstration of the scientific principles involved, i.e., scientific feasibility.

A good example technology is that of inertial confinement or laser fusion. Two major discoveries, that of the mechanism of nuclear fusion by Hans Bethe in the late 1930s and that of the principle of the laser by Townes and Schalow in the early 1960s suggest that the concentrated energy in laser beams could produce the high temperatures and confinement time needed to produce a fusion reaction capable of being harnessed and controlled for energy production. Design concepts[53] and crude cost estimates for electric power plants based on this fusion concept have been advanced during the last two decades. The fact that a fusion reaction can be induced by laser-induced initial confinement has been demonstrated. "Break-even" energy production (the attainment of more energy generated by the fusion reaction than consumed in initiating it), however, has yet to be demonstrated, and this engineering feasibility demonstration may still be several years off. Considerable theoretical work and hardware development have as a goal such a demonstration.

Other concepts for fusion, such as magnetic mirrors and magnetic confinement are slightly further along in this RD&D stage but are still in the scientific feasibility stage of scientific demonstration.

At the time of the selection of an AIS technology for uranium enrichment by the DOE (Spring 1982), the three candidate processes (AVLIS, MLIS, and PSP) had all attained scientific feasibility demonstration. The major question became that of determining whether they could work on a production scale and at what projected unit product cost? The winner of that competition, the AVLIS process, by virtue of better definition and understanding of the scalability issues, won that competition and was selected to proceed toward the engineering feasibility stage.

RD&D Level II: Engineering Feasibility Demonstration

The engineering feasibility stage is achieved when it appears that the major large-scale hardware necessary for an economic process is indeed developable in the near term and will be sufficiently reliable for use in a plant. All of the necessary systems may not be operating together, but the process integration issues are understood. The process hardware should be past the bench-scale development stage and should be close to a point at which it could be integrated into a pilot plant or subscale demonstration facility (the next stage of RD&D).

By way of examples, the overall AVLIS process is at the engineering feasibility stage. The lasers needed for separation of the U-235 isotope have been scaled to a size needed for a plant. A near full-scale chamber in which uranium vapor is to be generated and handled is nearing completion. The other uranium enrichment technology still under

development by the DOE, the AGC (advanced gas centrifuge) is also in the engineering feasibility stage and is competing with AVLIS for eventual deployment. Both the AVLIS and AGC have been extensively modeled and are continuously being assessed by the methodology here presented.

Another technology, which can be said to still be in the engineering feasibility stage, is the U.S. breeder reactor program. The Fast Flux Test Facility is the largest operating U.S. breeder facility but it demonstrates only a portion of the nuclear technology necessary for construction of a power production reactor. Construction of an integrated power production facility, the Clinch River Breeder Reactor Project, was halted in the initial construction stages.

RD&D Level III: Integrated Subproduction Scale Operation

Any pioneer process with an operating pilot plant can be said to fall in this category. At this point the basic science and process integration issues should be well understood and any remaining issues resolved by experiment. The important issue now becomes one of attaining enough process performance data to design and optimize a first production facility. After the data are obtained, a detailed conceptual design and cost estimate for a full-size plant or full-size production unit should be completed. If the results of the analysis appear economically attractive, this would probably be the point at which a decision to build the first large-scale facility would be made.

Examples of process technology in this stage are numerous. Nearly any new chemical process must complete this development stage. In the energy area, such diverse processes as fluidized bed coal combustion, flat-plate solar collector power plants, and many synthetic fuels

production plants fall in this class. Most of the chemical and synfuels processes mentioned above utilize conventional chemical engineering unit operations in their process steps.

RD&D Level IV: First Large-Scale Facility

These first-of-a-kind or pioneer process plants represent the culmination of an RD&D program. The period encompassing the integrated subscale facility stage (III) and this stage (IV) may have included the generation of two or more detailed cost estimates. These would represent the AACE class 3-5 estimates discussed in Chapter III. The Rand study[54] cited in Chapter III utilized processes in this class for its data base on actual plant capital costs and performance. For predicted costs and performance Rand cited estimates made when the processes were in RD&D Levels III or IV.

Among the types of process facilities at this stage are most synthetic fuels plants, the Gas Centrifuge Enrichment Plant (GCEP), an enrichment facility being started up in Portsmouth, Ohio, and the Fort Saint Vrain gas-cooled power reactor in Colorado.

RD&D Level VI: Processes Reduced to Practice

At this point the problems with the first plant have been resolved and additional plants may be slightly revised duplicates of the first. Such plants can often be ordered and constructed with nearly all RD&D and engineering tasks already accomplished. Most industrial facilities fit this mold, such as oil refineries, gaseous diffusion plants for uranium enrichment, and steel mills. Some facilities, such as light water nuclear power plants (LWRs), fall between Levels V and VI. It is true

that LWR technology is reduced to practice; however, in current practice each plant is designed for a given geographical site, set of seismic criteria, and environmental regulations. In some sense each LWR becomes a first-of-a-kind project. This problem contributes greatly to LWR costs and is discussed in an article by the Hellmans.[55]

It should again be noted many certain processes will fall between these RD&D levels. The next section will show a matrix diagram that can be used to demonstrate how the RD&D status of one process can be compared to that of another.

The Process Function-Development Status Matrix

The question of when to apply this economic evaluation technique and to what processes it can be applied is made more clear by use of a two dimensional matrix as shown in Figure 4.4. The ordinate variable represents a breakdown of the Level 4 category from the technology morphology discussed in subchapter IV-1.1. Levels 4-A and 4-B designated whether a process was a labor-intensive manufacturing process or a transformation process, respectively. In reality there exists no clear boundary between these two designations. The ordinate of Figure 4.4 is designed to reflect the extent to which the value added to the product commodity is derived from transformation as opposed to manpower-intensive steps. Processes which consume a large amount of energy or utilize large quantities of expensive raw materials would appear toward the top of the matrix. Processes for which a large proportion of the unit cost is derived from the cost of labor would appear low on the matrix. On the abscissa is plotted the RD&D status level of

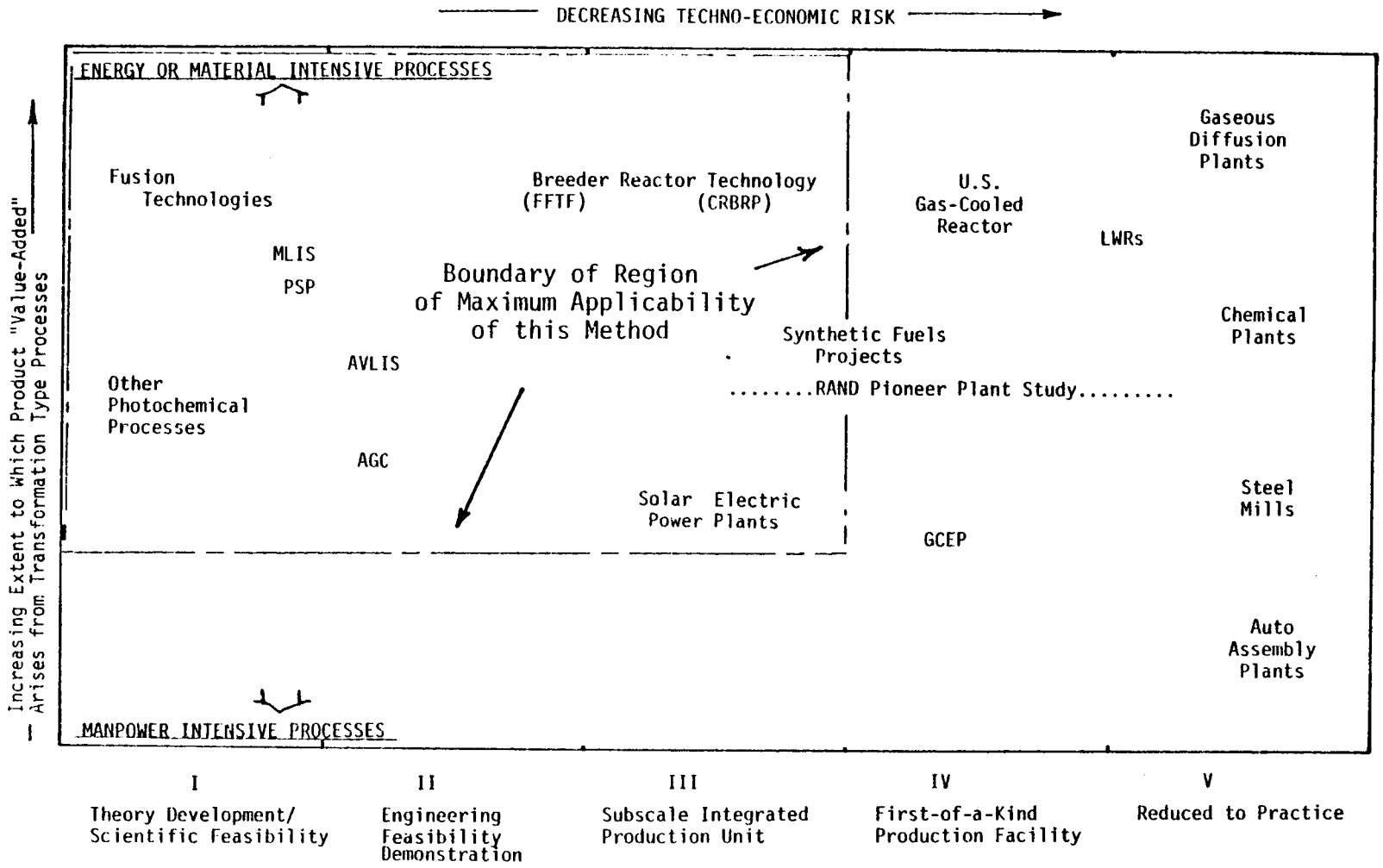


Figure 4.4

The Process Function/ Development Status Matrix

the process, with less developed processes such as fusion appearing on the left. Processes reduced to practice appear on the right. Several projects and technologies are shown on this matrix, many of which represent new processes based on recent technological advances. All of the uranium enrichment technologies evaluated by the DOE and its contractors are shown, including those which were not selected (MLIS and PSP) in 1982. The matrix is most useful for determining the applicability of this economic evaluation technique and for discussion of the limitations of the Rand methodology (discussed in Chapter III) for predicting cost growth and performance degradation.

This methodology is most useful in the mid to upper portion of the left-hand 60% of the matrix diagram. These processes are in or between the theory development/scientific feasibility stage (Level I), the engineering feasibility (Level II), and the integrated subproduction stage (Level III). These processes can best be described and modeled in terms of their constituent physics, chemistry, and design equations. The cost of labor normally does not represent a large percentage of the unit production cost. This methodology, however, does not ignore how one treats the problem of calculating labor requirements and staffing. The method's primary orientation is devoted toward correct representation of the process science and its impact on process design and costs.

It is also useful to bracket the region in which the Rand study[56] data base was located, i.e., transformation processes in RD&D stages III through IV. As can be seen from the matrix, the regions of applicability for this methodology and Rand's method only partially overlap. This again suggests that predictive use of the Rand algorithms for cost

growth and performance degradation may be very hazardous for processes in early (RD&D Levels I and II) development stages.

Financial and Temporal Scope of Project

This methodology is best applied to process development projects which are large in scope, i.e., incur development timelines on the order of several years and involve very significant monetary investments in both the R&D program and the life cycle of the production facility.

A typical R&D program might span 5 to 12 years and the production facility deployment, construction, and start-up project might span an additional 5 to 10 years. The operating project, during which levelized production is assumed, might span 15 to 40 years. For some energy technologies, such as fusion, the R&D program may span decades. The payoff or necessity for such long-term expenditures must be very high, and the Federal Government is often the prime sponsor of such efforts. Short-term R&D programs, such as those often encountered in the specialty chemical industry, often span only a few months and do not warrant full application of the methodology discussed here.

The total capital costs for the project to be evaluated should be of order of magnitude $\$10^6$ or larger. Since no more than 1% of the projected project capital costs should be spent on evaluation, and a reasonable short-term evaluation effort will cost at least $10,000, the above minimum figure of $\$10^6$ is reasonable. The evaluation cost should include the salaries of analysts and engineering estimators along with computing costs.

During the R&D program, the economic evaluation costs are often

included as part of R&D costs. For this case there is no rule-of-thumb which should dictate a particular fraction of R&D costs to be spent for evaluation.

Once these fourfold questions concerning the nature of the application are understood, the user should quickly be able to determine the applicability of the method. If the answers to two or less of the four questions indicate that this method is applicable, another methodology of evaluation is probably superior. If three of the criteria are met, it is likely that at least a significant part of this methodology may be useful. If all four criteria are met, the user should proceed to the next step of determining whether the project modeling objectives are sufficiently similar to those of this methodology that he or she can proceed with the modeling steps described in the two chapters which follow.

Nature of the Modeling Tasks, Uncertainties, and Figures of Merit

At the end of Chapter I three evaluation tasks were outlined along with the types of models and the types of uncertainties appropriate to each. In order to utilize this methodology the user must verify that task II (process assessment) is the objective and that technological uncertainties are of most interest. Strategic uncertainties (such as interest rates, deployment schedule, and production campaign length) may still be important; however, they may be best handled by a different model in a separate uncertainty analysis. Two good examples of strategic uncertainties analyses are the original investment analysis application of Hertz[57] and a project scheduling uncertainty analysis

of Owen and Nabors.[58] If the user determines that he is more interested in a task I application (Development Planning), there are special software packages such as GERTS[59] which can expedite the decision modeling task.

For early task II models, which are often several years prior to deployment, technology related figures of merit are appropriate. The unit cost of product (product in this case can be an energy or material commodity) is preferable since it includes total annualized costs and performance in the same aggregate figure of merit.

It also represents a very useful figure of merit for the unique process reoptimization feature which constitutes an important part of this methodology.

Other figures of merit, which can often be calculated simultaneously, are the total capital cost (sometimes called the total estimated cost or TEC) and the levelized annual operating cost. If the user wishes to utilize other figures of merit, he can build them into the task II assessment model.

The Monte Carlo uncertainty analysis technique itself is applicable to any model or figure of merit, hence the basic simulation methodology described in Chapter VII requires few alterations, regardless of whether task I, II, or III is addressed. The nature of the input variables supplied to eash task, however, will be markedly different.

As the user proceeds into Chapters V and VI, it will become apparent that sufficient flexibility exists in this methodology to assess a wide variety of new processes and their associated cost and technology related figures of merit.

CHAPTER V

PERFORMANCE AND DESIGN ANALYSIS

Preface

Once the user has determined that this methodology is suitable for economic evaluation of his process, the model building task should commence. What is now a set of technical concepts and hardware requirements must now be translated into mathematical algorithms suitable for uncertainty analysis. At this point the user may already have participated with development in performing some preliminary design calculation which may already provide a starting point for analysis; however, such a detailed previous analysis by the economic evaluator is not a prerequisite to begin the modeling effort. It is presumed that the development organization will be able to supply most of the necessary preliminary process information.

The performance and design models developed will be process specific, however, a special format for their construction, which is drawn from process control concepts, will be presented along with appropriate examples.

In addition to adherence to the modeling rules, however, educated judgments and considerable intuition on the part of the analyst are required. Familiarity with or access to the elements of the process science or "theory" and the proposed process design requirements are necessary to understand the relationships between the performance and design modules which constitute the transfer functions describing the process.

Four steps are required for construction of the appropriate performance and design models. These are:

(1.) Generation of an initial design concept, i.e., an initial reference case (with the help of process development staff members). This case may not necessarily be optimized for minimum unit cost of product.

(2.) Determination and categorization of the modeling variables.

(3.) Construction of connected performance, design, and cost models in a deviation/transfer function/response (DTFR) format capable of redesign and reoptimization of cases in which input variables deviate from the reference case values.

(4.) Generation of an optimized baseline process for further model refinement. This task also demonstrates to development staff that the optimization done by the model is acceptable and results in a minimum unit cost of product.

Each step will be discussed generically at first, followed by application of the four steps to a simplified hypothetical process. Figure 5.1 shows the contributions that each part of the overall organization must supply to begin the modeling task.

Generation of an Initial Design Concept

Before modeling of a process can begin, management and the development organization must supply the user of the methodology with project goals and a process concept. For many projects, this may take the form of "back-of-the-envelope" calculation or a few sketches with appropriate calculations. At this point, engineering cost estimators probably have

STEP	MANAGEMENT	DEVELOPMENT	COST ESTIMATING AND ENGINEERING	ECONOMIC EVALUATION
1. Initial Concepts	Specify desired annual production, scale of application, figures of merit.	Determine variables which define reference process.	Develop "best guess" cost estimates for unique major hardware items and significant operating costs.	Conceptualize model about reference process design.
2. Determination & Categorization of Modeling Variables		Determine which variables are uncertain.		Assist dev't. in determination of uncertain variables. Decide which variables are model inputs and which are variables to be utilized for redesign and reoptimization.

Figure 5.1

Data Sources and Organizational Functions Required
to Support the Modeling Effort

STEP	MANAGEMENT	DEVELOPMENT	COST ESTIMATING AND ENGINEERING	ECONOMIC EVALUATION
3. Model Development			Assist economic evaluators in development of cost scaling relationships.	Construct modeling algorithms in deviation/transfer function/response format with redesign and reoptimization capability.
4. Generation of Baseline Process Estimate		Supply "best guess" variable values which define optimized baseline process.	Re-estimate optimized baseline in more detail to support further cost scaling.	Utilize assessment model to determine optimized baseline.

Figure 5.1 (Continued)

not been involved except perhaps for the generation of cost estimates for a few major hardware items. Included in the information the modeler must have at his disposal are:

(a.) Scale of application. The desired productivity of a plant.

(b.) Figure of merit. The figure of merit for process optimization must be determined in advance. For processes in this early R&D stage, the unit cost of product is appropriate, since both performance and capital and operating costs are included in its calculation.

(c.) Process definition. The process physics and chemistry concepts which relate process productivity to equipment geometries, yields, efficiencies, operating conditions, and energy requirements. The theoretical or experimental data supporting estimation of productivity.

(d.) Process hardware technology. Performance specifications for the major hardware items, especially those which are first-of-a-kind or novel items, required for a production process.

(e.) System interactions. The logic of arranging the process steps into a workable process system.

(f.) Estimates of capital and annual operating costs. A preliminary best-guess cost estimate for major hardware items. A rough projection of annual operating costs, e.g., labor, material, and utilities.

In any case, even a very limited design and costing effort is needed prior to application of the methodology in order to establish the reference process upon which significantly more detailed economic and

performance modeling and evaluation can be built. A cost estimating engineer working with the development team and possible hardware suppliers should be able to provide much of these preliminary data to the economic analyst. Preliminary capital and operating cost data are also needed for purposes of optimization, as will be shown. This type of preliminary design scoping exercise has been performed for many process technologies, several of which have been discussed in the open literature [including laser isotope separation,[60] and laser-induced (inertial) fusion[61]]. Proposed processes or technologies often discussed in the MIT Technology Review[62-65] or the Scientific American[66] have often been evaluated at this preliminary stage. For nearly all such processes, no commitment to the construction of a production facility has been made.

It should be noted that such preliminary designs and cost data often represent single-point, optimistic, "best-guess" estimates; and the unit cost of product is usually unoptimized with respect to the important process variables. Such development-generated data, however, must form the basis for the modeling steps to follow.

Determination and Categorization of Process Variables

Internal and External Variables for Connected Models

The overall process assessment model must encompass three connected sub-models or modules: process performance, process design, and production costs. This chapter will consider mainly the first two of these, saving the details of the third module for the next chapter. It is necessary, however, to bring a generic discussion of cost into this

chapter, since optimization of the process is accomplished by minimization of the unit product cost and is a crucial part of this methodology. The tangible factors which influence the figure of merit that the overall model calculates (in this case unit cost) represent the modeling variables. Some variables are supplied directly as input to the overall model, and others are passed between the three modules of the overall model. Figure 5.2 illustrates this schematically and refers to the input array, X_i, as externally supplied variables, and those passed between modules, array Q_i, as internally generated variables. Table 5.1 also shows the sub-arrays into which these variables can be classed and gives examples of each. Typical input variables would constitute the development determined coefficients and certain externally controlled operating conditions for the process. Internally generated variables include calculated quantities such as yields, material balance streams, and design data.

The general flow of information in Figure 5.2 is from left to right, i.e., performance to design to cost. It will be seen that optimization of the process will require that unit cost information be returned to earlier model modules.

Model/Variable Relationships

The performance model calculates the productivity, P, of the process for the external set of operating conditions, X_i, supplied to it and also passes design requirements (part of the Q_i array) to the design model. The operating conditions are derived from the performance input variables, $(X_i)_{perf}$, and any internally generated variables, $(Q_i)_{fb}$, fed

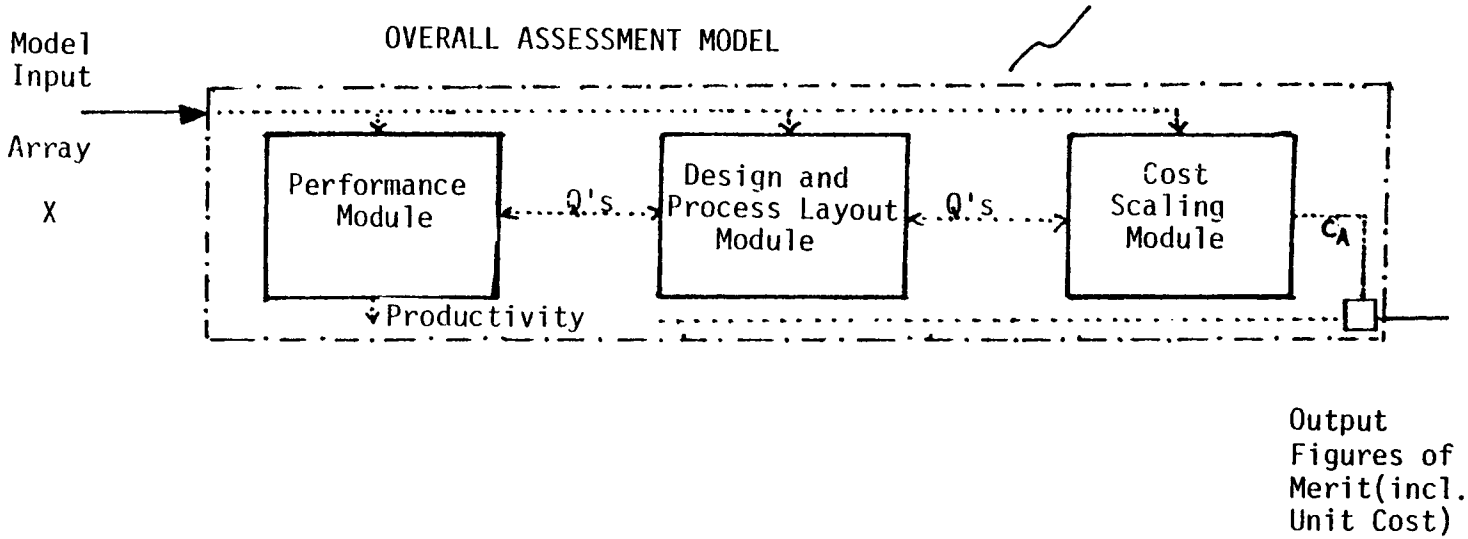


Figure 5.2

Modular Structure of a Process Assessment Model

Table 5.1

Categorization of Generic Modeling Variables X_i and Q_i with Examples

Input Variables		Internal Variables	
X_i Type	Examples	Q_i Type	Examples
$(X_i)_{perf}$	Uncertain Operating Conditions Atomic and Molecular Data Kinetic and Equilibrium Data Uncertain Material Properties	$(Q_i)_{perf}$	Yields, Conversions Power Consumed
		$(Q_i)_{des}$	Flow Rates and Material Balance Equipment Sizes Energy Balances
$(X_i)_{des}$	Efficiencies Scaling Parameters Load Factors Limits on Equipment Sizes		
		$(Q_i)_{fb}$	Equipment Geometric Configurations Conversion Pressure and Temperature
$(X_i)_{cost}$	Unit Hardware Costs Energy Unit Costs Learning Rates Feed Costs Reliability Data		

back from other parts of the model (such as an optimizer in the design model).

The design model sizes the major process equipment as a function of the requirements supplied by this performance model, $(Q_i)_{perf}$, any design related externally supplied input variables, $(X_i)_{des}$, and any internally generated variables fed back from other parts of the model $(Q_i)_{fb}$. In addition to equipment sizing, the design model lays out the equipment on the process floor and specifies a building and site size to envelop the plant facilities.

The cost scaling model performs the task of a cost estimator by calculating plant capital and operating costs as a function of equipment size and plant operating conditions calculated by the design model, $(Q_i)_{des}$. Other inputs, $(X_i)_{cost}$, such as unit hardware costs or reliability data, are supplied externally. The total annualized cost, C_A, constitutes the major output of this model.

The variables denoted as $(Q_i)_{fb}$ are controllable or alterable quantities (as a result of a feedback mechanism) which are utilized in the optimization of the process via the performance and design models.

Qualitative Selection of Input Variables: Information Sources

At this point the modeler should not be concerned with variable numerical quantities, but rather the qualitative question of what are the variables, i.e., the important unit cost determining factors? The R&D organization should be familiar with many of those factors which drive process performance, and will probably have performed one-variable-at-a-time, i.e., single value sensitivity studies (SVSS), on their own to make this determination. For a new process there will

usually be two to twenty such performance- and cost-driving variables. It is the task of the modeler to mathematically represent unit cost figures of merit in terms of these variables and incorporate them in the three modules discussed above.

The user must also ascertain from development which variables are likely to have the most uncertainty. In categorizing the variables it is important that these uncertain variables be considered as input variables, X_i, supplied external to the model, since the Monte Carlo driver code will later be used to select ensembles of these variables from probability distributions.

Categorization of Variables

The modeler must mentally conceptualize the process and decide how he wishes to treat different types of variables. The modeling algorithms will consist of the two classes of variables discussed previously, the X_is or externally supplied input variables [which can be divided into subclasses: performance, $(X_i)_{perf}$; design, $(X_i)_{des}$; and cost, $(X_i)_{cost}$], and the Q_i or internally generated variables which are subclassed into performance, $(Q_i)_{perf}$; design $(Q_i)_{des}$; and feedback $(Q_i)_{fb}$ variables. The latter subclass $(Q_i)_{fb}$ represents the iterated variables which will be utilized to redesign and reoptimize the process for any given set of values for the input variables, X_i. The modeler must determine in advance which of the Q_i variables will perform the crucial redesign and reoptimization function.

A reference array of numerical values for the process input variables, $(X_i)_{ref}$, represents a given set of conditions which development feels adequately represents the process. Each variable value in

$(X_i)_{ref}$ represents development's "best-guess" value for the reference case. It is important for this reference case and any other case, i.e., a different set of X_is, which may be derived from further development work, that the unit cost of product, C_U, be optimized with respect to the changeable internal variables, $(Q_i)_{fb}$.

Framework for Model Construction

Models as Transfer Functions: A Process Control Analogy

As mentioned earlier, the performance and design models are highly process specific. One cannot write design and performance algorithms suitable for all processes, since any given process will be based on different physical or chemical phenomena.

Given the input variables, X_i, the internal optimization variables $(Q_i)_{fb}$, and the unit cost figure of merit, C_U, for a given process, however, one can impose a strategy or modeling framework which can guide the user in the model construction process.

The key is that the user think of the set of algorithms in the three modules (performance, design, and cost) as constituting an extremely complex transfer function or input/output function with a feedback loop to handle reoptimization. The concept of transfer functions is taken from process control, and the analogy is appropriate, since in essence it will be shown that a process model can be developed in which the performance (i.e., productivity) is self-correcting. Degraded process performance, the result of deleterious changes in process inputs, can be offset by changing some of the operating conditions, adding more process equipment, or increasing the size of the reference design equipment.

In the simplest form, the transfer function can be represented as a single block in which the inputs are the variables, X_i, and the output or response is the figure of merit; i.e., unit cost of product, C_U. At the time modeling begins, development can supply a set of best guess inputs, $(X)_{ref}$, which correspond to a reference projected value for the unit cost $(C_U)_{ref}$. In control theory this is analogous to an initial steady state and a set of variables $(X_1)_{ref}$, $(X_2)_{ref}$, $(X_3)_{ref}$, etc., for which $(C_U)_{ref}$ would be related by the algorithms in the transfer function. For purposes of uncertainty determination, however, one must deal with deviations or ΔX_i from these reference or "steady-state" values. Such deviations result from newly obtained development data concerning the values of the inputs, X_i, and the possibility that alternative values $X_i \neq (X_i)_{ref}$ might exist. In many instances, further development work indicates that a given X_i may no longer have the value $(X_i)_{ref}$ originally proposed. The transfer function (via its constituent algorithms) must be able to calculate the new value of the unit cost, $C_U \neq (C_U)_{ref}$, resulting from this new development information.

In control theory this is analogous to calculating the new steady state resulting from a deviation in a value of X_i. In control applications, X_i is a function of time, and one is interested in calculating how long the figure of merit (usually called the response) will take in reaching the new steady-state value. For the present application recovery time is not of interest or meaningful; hence, only "steady-state" calculations will be compared. Dynamic simulation, in which time is an important variable, represents a modeling technique with a different purpose; i.e., one related to later RD&D stages. A paper by White[67]

discusses a typical dynamic analysis application. It is important to understand that the objective here is not actual control of an existing process or simulation in time of a proposed process, but rather redesign and reoptimization of the process. Figure 5.3 should clarify the analogy to process control transfer functions.

In most control applications, a feedback loop exists for allowing rapid recovery of the process to a steady-state condition. The value of an output variable is fed back to a controller, which in turn resets variables internal to the transfer function. Figure 5.4, which represents a more detailed subdivision of the simple transfer function in Figure 5.2, shows that an analogous feedback mechanism can be built into a process model. The intent is not to control the process in the conventional hardware sense, but via process design and reconfiguration to allow the process performance to recover from deviation in one or more input process variables, X_j.

The Redesign Requirements

Since management and development have specified a desired productivity, P_o for the process, the transfer function (performance and design models) must be capable of reconfiguring the process to attain P_o for one or more $X_j \neq (X_j)_{ref}$. By allowing selected internally generated variables, Q_j, to change, a new design along with new associated costs is generated. Thus a new value for the total annualized cost, C_A, and the unit product cost, C_U, is calculated.

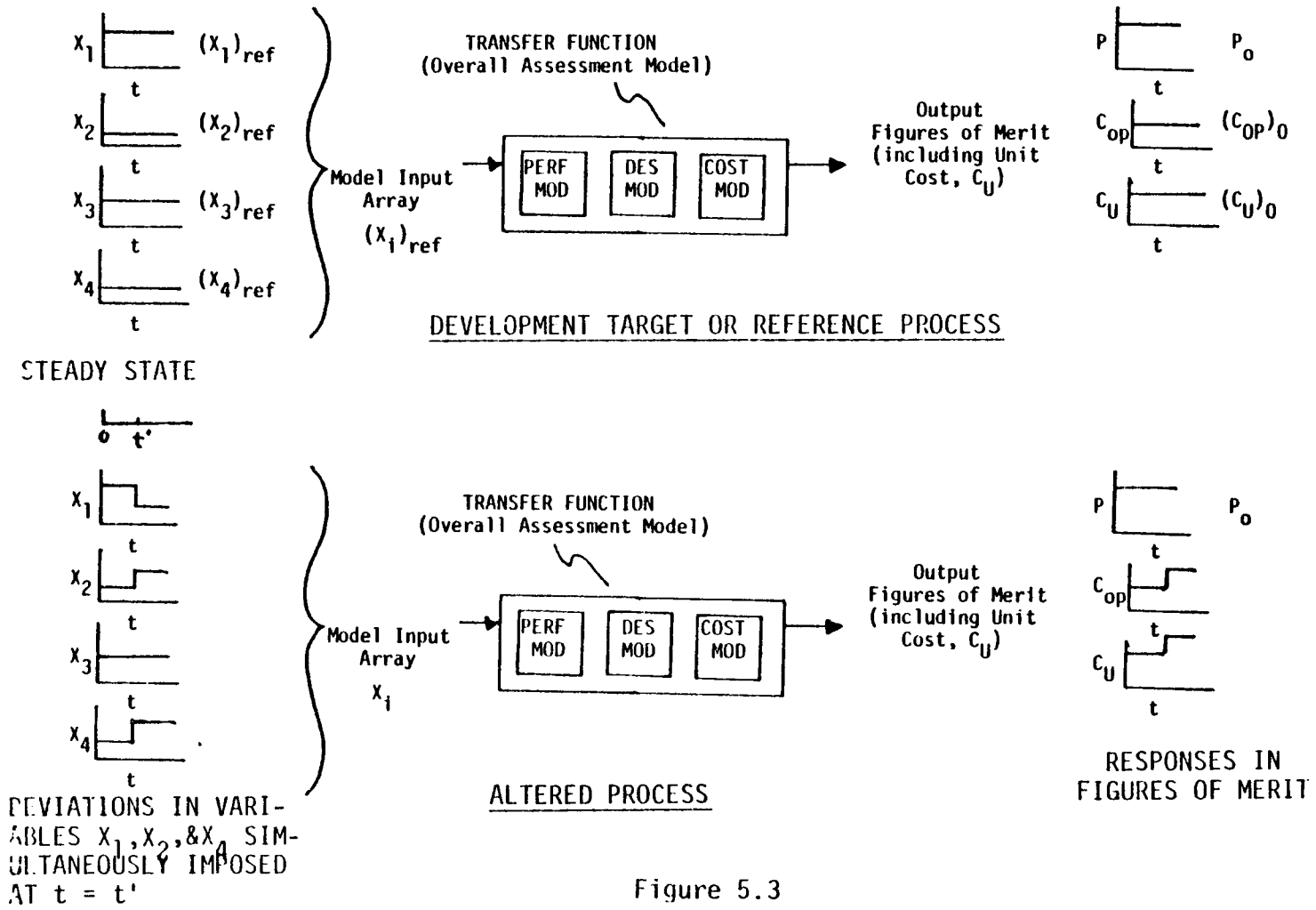


Figure 5.3

Deviation/Transfer Function/Response Analogy for Construction of Assessment Model

i = Identifier for Q or X variable
j = Index for optimization iterations

This case has: 9 input variables (X)
4 feedback or optimization variables $(Q)_{fb}$
8 other internal variables $(Q)_{perf}$ or $(Q)_{des}$

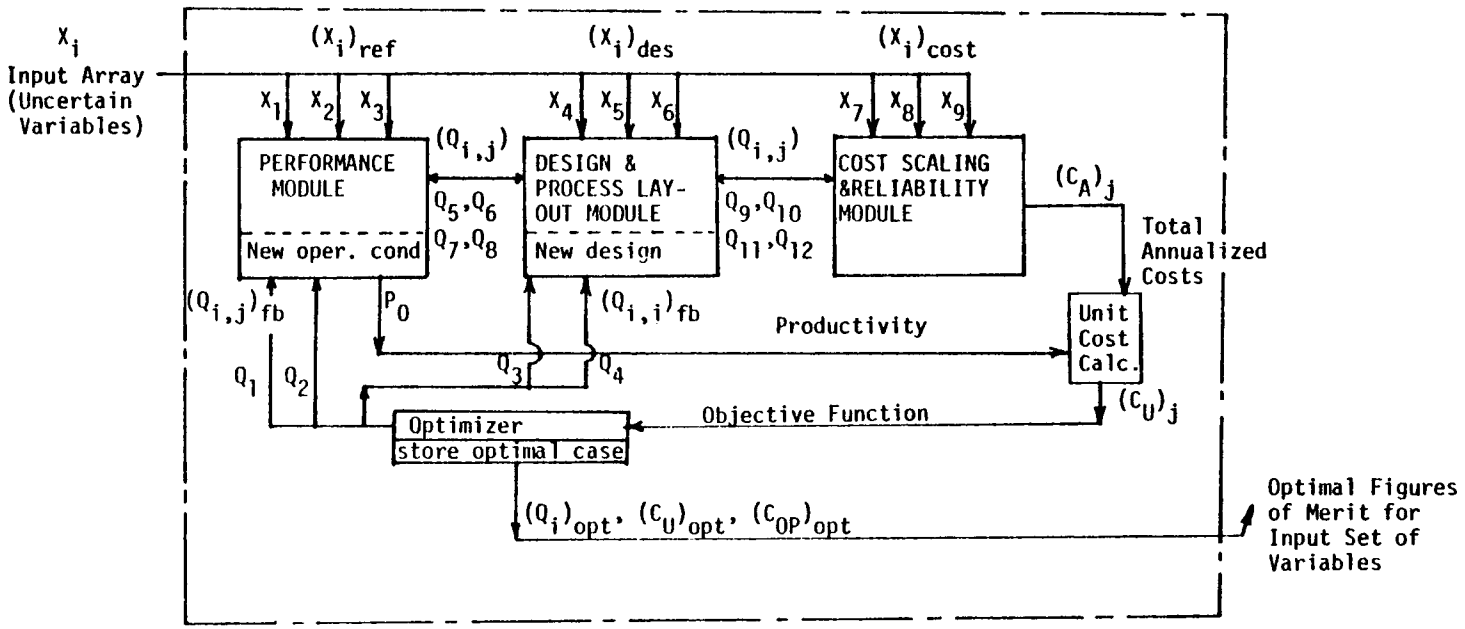


Figure 5.4

Schematic of Redesign and Reoptimization Features of Assessment Model

The Reoptimization Requirement

For each set of inputs, X_j, defining a non-reference case, it is possible to optimize the unit cost, C_U, with respect to the variables $(Q_i)_{fb}$ available for optimization. The unit cost calculated by transfer function or model in this case is the objective function. This procedure requires that an iterative grid search or other optimization technique be invoked for each new non-reference design examined; however, it assures that the new process configuration generated by the redesign feature above is physically reasonable and unit cost-minimized. For each set of inputs, X_j, defining a particular case, it is necessary to calculate the unit cost, C_U, for each optimizer iteration; since the optimizer must search for the minimum $C_U = (C_U)_{opt}$ and save the set of internal variables $(Q)_{opt}$ which corresponds to the optimal case.

The Cost Model Requirement

It should be noted that some form of cost scaling model is needed for determination of the unit cost objective function. During development of the process performance and design models and initial design and optimization of the process, the cost model can be very simple and only consider a few important cost scaling relationships. Detailed modeling must await this generation of an engineering cost estimate that includes all process-related items, such as buildings, process support equipment, staffing, and utilities. Only a few cost scaling algorithms are appropriate at this point, and the next chapter will consider costs in some detail.

Process Redesign Procedure

Calculation of new designs for non-reference inputs $X_i \neq (X_i)_{ref}$ requires that the model have built in the capability to recover from degradations in productivity. Suppose as a result of X_1 changing from $(X_1)_{ref}$ to $(X_1)_{off}$, the productivity calculated in the performance model drops from $(P_o)_{ref}$ to $(P_o)_{off}$. By comparision of $(P_o)_{ref}$ (desired) and P_{off}, the modeler has two options for restoring P to its previous nominal $(P_o)_{ref}$. He can instruct the modeling algorithm to either:

(1.) Specify an increased number of production units of the reference size. (This technique is useful where small production units are installed in parallel.) Such units might be gas centrifuges, solar-cells, lasers, or heat exchangers of a given reference size and capacity.

(2.) Specify scaled-up units to compensate for the production short fall. This technique is useful where only one or a few units are required (i.e., reactor cores, chemical reactors, and generators) which can be designed to fit the plant's requirements.

The consequence of such new designs are likely to be increased capital and operating costs; however, reoptimization of the unit cost for each case will at least minimize these additional costs. If the changes in the inputs produce beneficial results, i.e., $P > P_{ref}$, the model should have scale-down capability and the total annualized costs associated with P_o should be less than $(C_A)_{ref}$.

The method by which process redesign is accomplished depends on the nature of the process itself. The user must know enough about the

details of the process that he can instruct the model to reconfigure the plant such that the model will automatically compensate for possible shortfalls in the performance of the major hardware items.

Generation of an Optimized Baseline

In order for more detailed cost estimating and process cost-scaling activities to proceed, a single point, "best-guess", or baseline projection must be generated. It is presumed that the performance and design modules have been constructed per the previous step and that any one case representing a given set of input variables, can be optimized with respect to the appropriate internal variables, Q_i, such that a minimum unit cost results.

The development organization must now be again asked to supply their latest best guess as the values of the input variables, X_i. For this set of values, $(X_i)_{base}$, called the baseline ensemble, an optimum set of internal variables $(Q_i)_{base}$ can be found which results in the minimum unit cost, $(C_U)_{base}$.

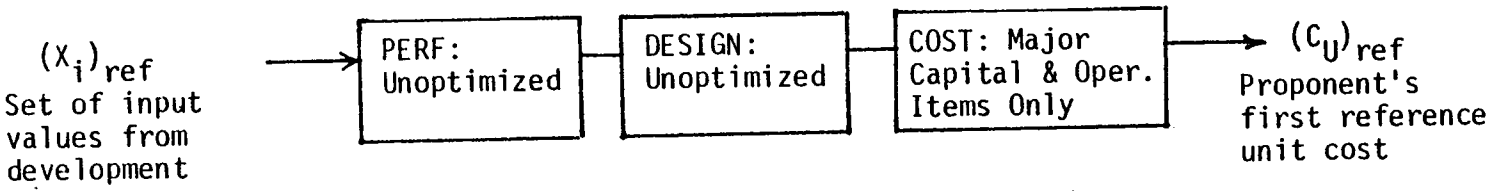
The design requirements, $(Q_i)_{base}$, which constitute this case now become the baseline reference for more detailed cost estimating. The requirements include major material balances, the duties for major hardware items, equipment sizes, and energy requirements. As will be shown in the next chapter, cost estimates made for designs incorporating these baseline requirements serve as the pivot points or bases for the construction of more detailed cost scaling equations. During this next cost estimating task, hardware items other than the few major cost drivers will undergo cost estimation. Such items include support

facilities, buildings, balance-of-plant items, and other annual operating costs such as plant staffing.

From this more detailed design task a new annual production cost, $(C_A)_{rev.base}$ [and unit cost, $(C_U)_{rev.base}$], corresponding to the baseline requirements $(Q_i)_{base}$ and baseline inputs $(X_i)_{base}$ will result which will likely differ somewhat from the less detailed costs embodied in the crude cost model originally used to optimize the reference design. The productivity and design requirements, however, remain essentially the same as the reference optimized case. This discrepancy in cost calculation arises because of the iterative nature of the overall performance/design/cost modeling exercise. Figure 5.5 illustrates the iterations involved over the course of a modeling effort. Because of the reoptimization feature, the three modules which constitute the overall model are highly interactive and involve the two-way flow of information in each. As a rule the calculation of performance and design must precede the calculation of costs; hence, the latest baseline design always tends to be optimized via a cost scaling module based on the previous cost estimating exercise. As more detailed modeling proceeds, the differences in the optimized baseline unit costs [for a given set of $(X_i)_{base}$] tend to diminish.

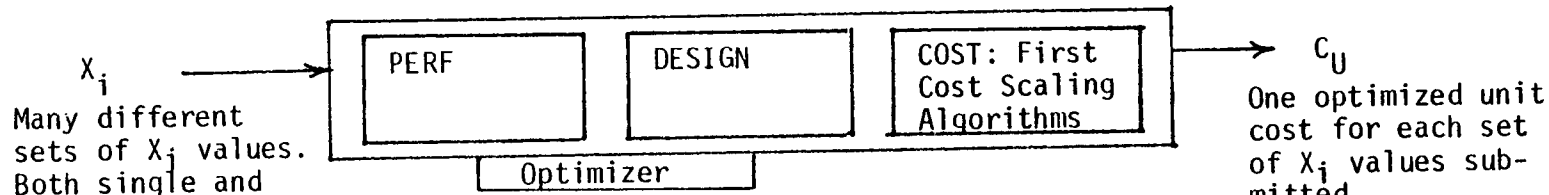
Before considering cost scaling, it is useful to reinforce the understanding of these abstract concepts via a simple example. For purpose of illustration the number of variables considered is few and the sample model very simple. If a real process were to be discussed at this point, the complexity of the models and number of variables would tend to obscure the demonstration of the model building methodology now desired.

① FIRST MODELING EFFORT (DEVELOPMENT)



- Model is not necessarily a computer code.
- Serves as basis for development of more sophisticated model for economic evaluation.

② MODEL DEVELOPMENT AND SENSITIVITY STUDIES (ECONOMIC ANALYSIS)

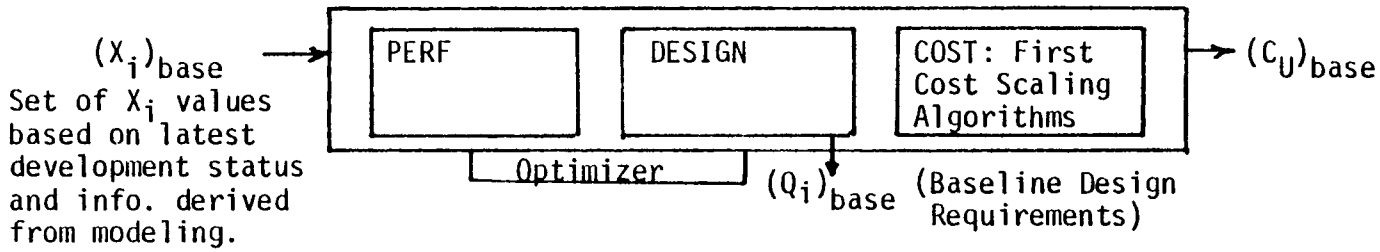


- Model incorporates redesign and reoptimization features.
- Model is a computer code.
- Model considers non-reference cases.

Figure 5.5

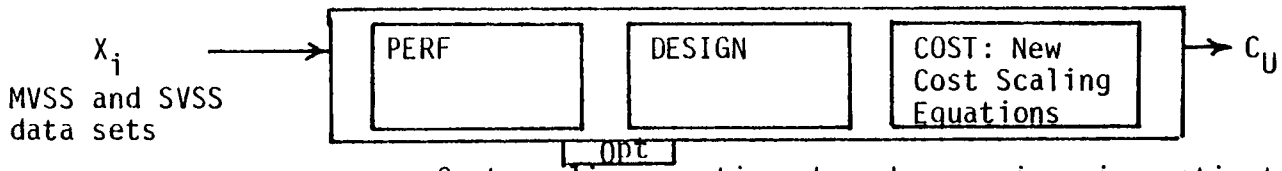
Iterative Nature of the Assessment Model Development Task

③ FIRST BASELINE DERIVED FROM MODEL IN ② ABOVE



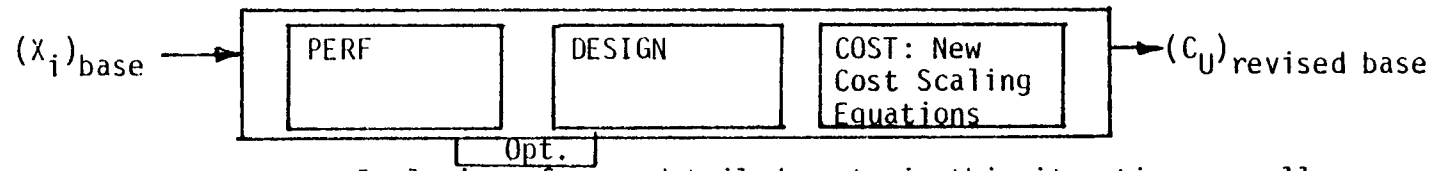
- These results serve as basis for detailed engineering cost estimate.

④ FURTHER MODEL REFINEMENT AND SENSITIVITY STUDIES



- Cost scaling equations based on engineering estimate and include BOP and process support items.
- Improved model used for these sensitivity studies.

⑤ GENERATION OF AN IMPROVED BASELINE PROCESS



- Inclusion of more detailed costs in this iteration normally causes $(C_U)_{revised\ base} > (C_U)_{base}$

Figure 5.5 (Continued)

The XYZ Catalyst: A Simple Case Study

Scientists and engineers employed by the XYZ Chemical Company claim to have developed a new catalyst that can effectively increase the rate of certain gas-phase reaction by a factor of ten. The desired compound "R," which the company wishes to eventually sell, is produced in a plug flow reactor of volume V by the following first order reaction.

$$A \xrightarrow{k} 4R$$

The catalyst is based on innovative use of a new material and has been tested in bench-scale laboratory equipment only. Sales of compound R could potentially be in the millions of dollars per year, and the development and testing of this radical new catalyst to produce R in large quantities could take up to 6 years. The cost of manufacturing the catalyst itself is also very uncertain, since development has only prepared enough of it to support bench scale production of small quantities of R. Based on initial development calculations, the tenfold increase in catalyst activity requires switching from the present catalyst/reactor system to a new simpler equipment configuration that promises to significantly decrease XYZ's annual production costs for a given quantity of R.

Based on the criteria discussed in Chapter IV, the process appears highly amenable to economic analysis by this method. It meets the requirements for description, RD&D stage, scope, and the evaluation task. The next step is to model the process in the form described in this chapter.

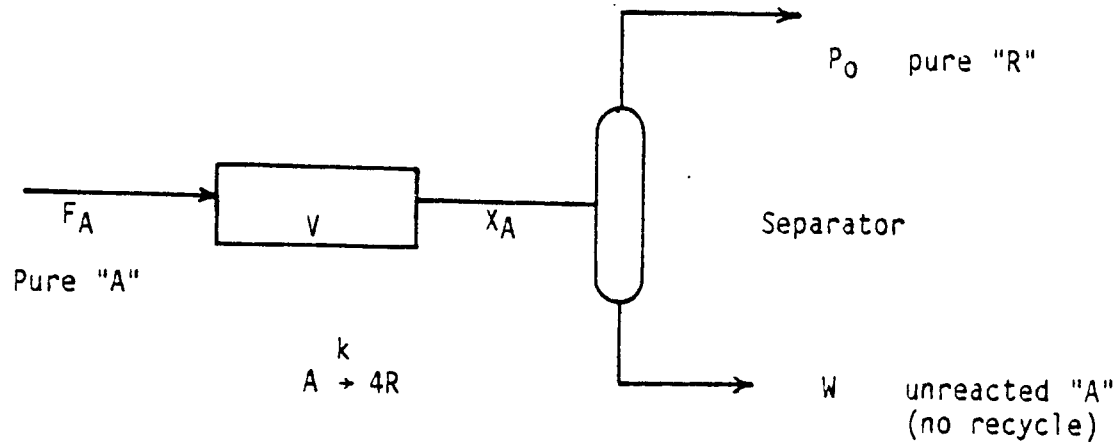
Step 1. The Process Concept

The plant here described will be assumed, for the sake of simplicity, to consist only of a plug flow reactor and a separation device which can completely separate R and any unreacted A. The following cost information for the development reference process is considered.

Capital Costs:	Reactor of volume V_o	C_{R_o} ($)
	Catalyst Load	C_{CAT} ($/g catalyst)
	Separator	C_{Sep} = 0 (for simplicity of example)
Operating Costs:	Feed Cost for A	C_{F_o} ($/gmol A)
	Other Operating Cost	C_{FIX} ($/year)

The reaction A → 4R is assumed to be first order and the rate constant, k, a direct measure of catalyst activity. The plug-flow reactor design algorithm and some of the process variables are derived from a differential reactor design calculation in Chapter 14 of Levenspiel's Chemical Reactor Engineering.[68] Figure 5.6 shows the reference schematic operating conditions and variables upon which the development organization believes a viable process can be based. The performance and design equations are also shown. A k value of 96 (liter fluid)/(hour)(liter catalyst) represents the development projected activity for the new catalyst. The desired productivity of 2800 gmol R/hour (24.5 x 10^6 gmol/year) is assumed to be specified by management. The 140 liter reference plug flow reactor for this case is assumed to cost $100,000 (without catalyst) and the catalyst is projected by development to cost $1/g.

Constant Pressure & Temperature
F,P,and W in gmol/hr



PERFORMANCE EQUATION or Module

$$P = 4 X_A F_A = P_o = \text{constant}$$

DESIGN EQUATION or Module

$$V = \frac{F_A}{k C_{Ao}} \left[(1 + E_A) \ln \left(\frac{1}{1-X_A}\right) - E_A X_A\right]$$

where:

- V = reactor volume (liters)
- F_A = feed rate of A (gmol A/hr)
- k = reaction rate constant [(liters fluid)/(hr)(liter catalyst)] (equivalent to activity for first order reaction)
- C_{Ao} = feed concentration (gmol A/liter of fluid)
- E_A = fractional change in volume of A upon reaction
- X_A = fractional conversion of A

Development Suggested Values (reference case)

$F_A = 2000$	$k = 96$	$P_o = 2800$
$C_{Ao} = 0.1$	$X_A = 0.35$	$C_{CAT} = 1.0$
$E_A = 3$	$V = 140.2$	

Figure 5.6

The XYZ Process: First Development
Reference Process

Step 2. Qualitative Variable Selection and Designation

It must now be determined which variables constitute internal variables, Q_i, and which constitute input variables, X_i. Development has stated that the eventual value of k in a production scale process is the most important performance driving variable, but that it is also highly uncertain since only bench-scale results have been obtained. The unit cost of catalyst, C_{CAT}, will be the predominant hardware cost issue. For simplicity, one can assume that the concentration of A in the feed, C_{AO}, will not change. The variable E_A is constant for the reaction of interest. By examination of the productivity and design equations in Figure 5.6, it can be seen that the conversion of A, X_A, and feedrate, F_A, determine the productivity. For a given k, one would like to find the combination of X_A and F_A that minimizes the unit cost of R. For this simple example the variables X_A, F_A, and V would represent internal variables, or Q_i values, for the model. Since X_A and F_A are directly related, i.e., $4X_AF_A = P_O$ = (constant), only one of the variables X_A or F_A need serve as the optimizing variable, i.e., a $(Q)_{fb}$ value.

Step 3. Model Construction in the Deviation/Transfer Function/Response Framework

The management and economic evaluation staff of XYZ Chemical Company are concerned about the possibility that the input variable, k may ultimately differ from the highly uncertain value of 96 obtained in bench scale studies. The modeler must now organize and construct the performance and design algorithm such that the productivity, P_O (2800 gmol R/hour) will be maintained regardless of the value of k.

If a degradation in k occurs, it can be seen from the design equation in Figure 5.6 that the two related factors, F_A and X_A, which affect productivity also affect the size, V, of the plug flow reactor required. To find the optimum unit cost, a preliminary cost algorithm, which balances the annual cost of additional feed against the annualized cost of a larger reactor, is required. This algorithm constitutes the third or cost module needed as part of this transfer function. Such a simple cost model might appear as follows:

feed cost	reactor cost	catalyst cost	other operating cost

$$C_A = 8760\, C_{F_0}\, F_A + C_{R_0} \left[\frac{V}{V_0}\right]^{0.6} f_{CR} + C_{CAT}\, d_{CAT}\, V\, f_{CR} + C_{FIX}$$

where:

C_A = total annualized cost ($/year)

8760 = hours/year

C_{F_0} = unit cost of feed A ($/gmol A)

F_A = feedrate of A (gmol/hour)

C_{R_0} = capital cost of reactor of size V_0 ($)

f_{CR} = capital recovery factor (1/year)

C_{CAT} = unit cost of new catalyst ($/g catalyst)

d_{CAT} = catalyst bulk density (g catalyst/liter reactor volume)

V = reactor volume (liters)

V_0 = reference volume reactor volume (k=96, X=0.35, F_{A0} = 2000 liters)

C_{FIX} = other fixed operating costs ($/year)

For the following reference values, a more simplified expression can be derived by combination of constant terms:

$C_{Fo} = 0.05$

$C_{Ro} = 10^5$

$V_o = 140$

$f_{CR} = 0.16275$

$C_{CAT} = 1.0$

$d_{CAT} = 5,000$

$C_{FIX} = 50,000$

By substituting the constants, this expression can be represented as:

$$C_A = 438\ F_A + 16275\ (\frac{V}{140})^{0.6} + 813.75\ V + 5000$$

We can now consider each of the three modules, which constitute the transfer function, and which for this example consists of one algorithm each:

Performance: $P_o = 4F_AX_A = 2800$ (constant)

Design: $V = \frac{F_A}{0.1k}\ (4\ \ln\ (\frac{1}{1-X_A}) - 3X_A)$

Cost: $C_A = 438F_A + 16275\ (\frac{V}{140})^{0.6} + 813.75V + 5000$

By examining the above expressions in block diagram or modular format as in Figure 5.7, the analogy to a transfer function becomes apparent.

For each value of k different from the reference value of 96, a deviation is represented. This new "forcing function" or k value causes the redesign feature and the optimizer to search for the value of X_A which results in a minimum value for the total annualized costs.

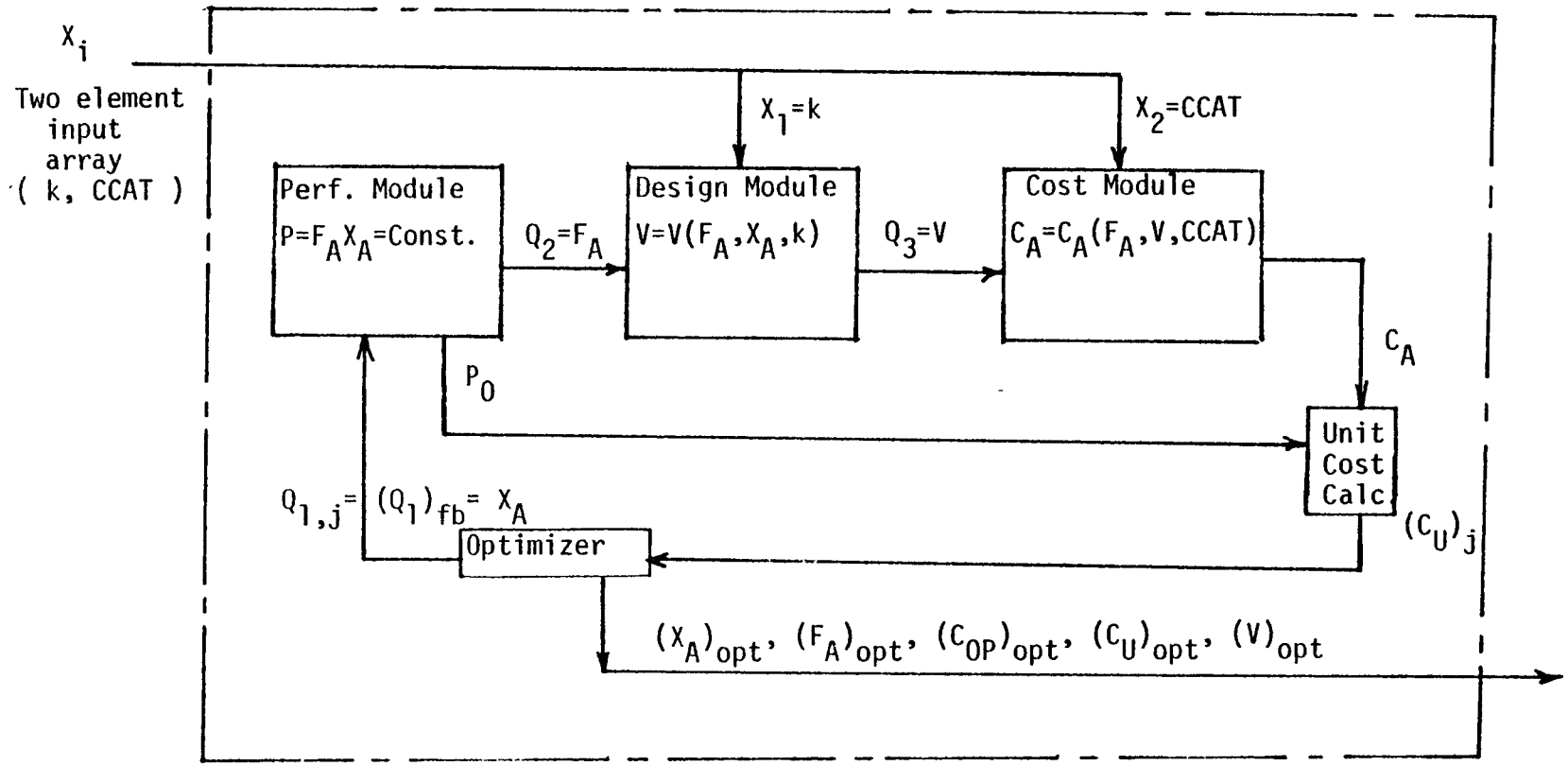


Figure 5.7

Modular Representation of the
XYZ Process

Since the desired P_o is constant and the unit cost is the ratio C_A/P_o, minimizing C_A is the same as minimizing unit cost, C_U. If k decreases, the design module will specify a new reactor size along with a different amount of feed, and via optimization it will balance the reactor capital cost against the feed costs such that their sum, the total annualized cost, is minimized.

A FORTRAN Model

Appendix E contains the FORTRAN model for the above calculation. The optimizer utilized is very simple and in this case consists of a single DO loop which iterates on X_A. If the variables and unit cost from each iteration are saved, the minimum production cost can be obtained by simple comparison of C_U values calculated. More sophisticated optimization techniques are available, which can more efficiently search for the optimum, however, they will not be discussed here. Optimization texts such as Smith, Pike, and Murrill[69] are suggested for descriptions of optimization algorithms.

Step 4. Optimized Baseline

The first column of Table 5.2 shows the developer's original unoptimized reference case which served as the basis for the model. When the optimization loop is utilized, it can be seen from the second column of Table 5.2 that different values of X_A, F_A, and V can be found (for the same k=96) which minimize C_U. This new set of values can be said to represent an optimized baseline and, since an economically superior design is projected, should represent the basis for further modeling efforts.

Table 5.2

Comparison Of XYZ Unoptimized And Optimized Developer Reference Cases

Variable	Unoptimized Reference Case Value	Optimized Reference Case Value
k $[\frac{l_f}{(hr)(l_c)}]$	96	96
P_o $(\frac{g\text{-mol R}}{hr})$	2,800	2,800
X_A	0.35	0.70
F_A $(\frac{g\text{-mol A}}{hr})$	2,000	2,000
V (liters)	140.2	282.9
P_{AN} $(\frac{g\text{-mol R}}{yr})$	2.45×10^7	2.45×10^7
C_{OP} ($/yr)	1,056,000	743,000
C_U ($/g-mol R)	0.0431	0.0303

The important result of the preceding is that the user now has an overall model that will calculate the economic effect of changes in uncertain variables and at the same time will force the design to somewhat compensate for any deleterious changes.

A single-value sensitivity study (Figure 5.8) on the activity k illustrates this point nicely. Figure 5.8 shows unit cost versus k curves resulting from both an optimizing and non-optimizing assessment model for the XYZ process. If a non-optimizing model is used, the resulting unit cost curve falls above that obtained if the optimizing model is used. For each off-reference (deviation) in k, the optimizing model more economically reconfigures the plant design.

The development organization of XYZ Company, as a result of the preceding modeling steps, will now have a better understanding of the economic effects of crucial process variables. The user of the methodology, the analyst, now has an optimized baseline from which the model can be improved and refined.

Comparison to Real Processes

The XYZ process here presented was greatly oversimplified. For a real process, each of the three constituent assessment model modules would consist of many algorithms of the preceding type. The number of input variables will also be much larger than one. The modeler must also assume that the input variables, X_i, are independent, i.e., one input variable does not automatically affect another. The model must be able to accomodate a multitude of different random combinations of possible X_i values for the simulation technique to be workable.

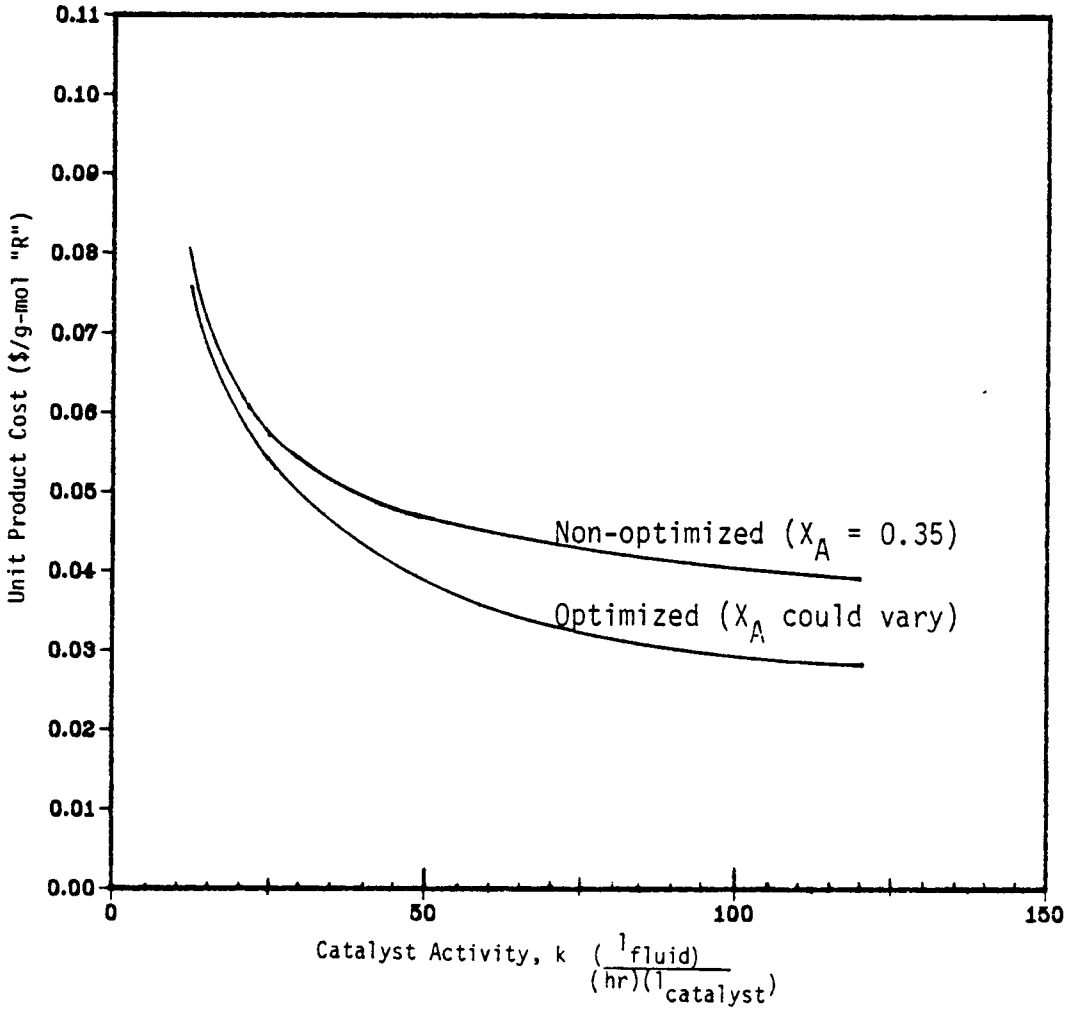


Figure 5.8

Effect of XYZ Catalyst Activity on Unit Cost of "R": Comparison of SVSS Utilizing Non-Optimizing and Optimizing Models

Some More Detailed Design Considerations

After an optimized baseline has been subjected to more detailed engineering design and cost estimating, the drawings and data sheets that result can form a basis upon which additional, more detailed design and cost algorithms can be developed. These algorithms mainly consider balance-of-plant and process support design requirements; however, reliability concepts such as availability and replacement requirements can be incorporated into the models at this point.

Availability Considerations

An important sizing issue for consideration in the design model is that of process on-stream fraction or availability. For some processes the modeler will face a decision whether to specify a larger processing unit or additional units of a reference size in parallel. Each option has its advantages and disadvantages. Large units often benefit from economics of scale; however, if a single unit fails, a large fraction of the plant is out of service. The redundancy afforded by smaller units often leads to higher plant on-stream time of availability which sometimes outweighs the cost advantages of large equipment. As will be discussed in the next chapter, availability is tied in closely with process component reliability.

Support Equipment Sizing

Where possible, conventional handbook-type procedures or equations are used to size equipment which fits the duty requirements imposed by the performance model, especially for conventional plant support items

such as piping, valves, heat exchangers, cooling towers, and transformers. In many cases the duty or capacity for a piece of process equipment encounters physical constraints on equipment size and performance, hence replication of equipment and use of parallel units are necessary.

Scaling in Facility Layout

Once the sizing of the major process and balance-of-plant items is complete, the items must be laid out in some logical floor plan such that the process equipment can be enclosed in a building if one is required. As process equipment designs vary from the estimated baseline, their projected floor dimensions (normally length and width) will also vary. Human factors engineering and logistical considerations mandate fixed aisle spaces, door locations, equipment access space, and operations staging areas; therefore, the total building area or volume must have sufficient additional space added to that specified for process equipment. In general, however, the size of the equipment or number of process units will drive the building area. For example, if a powerhouse requires 20% more generation capacity over the baseline power production process, one must either use 20% more production units (if small parallel units are used) or install a 20% larger unit, which will have larger dimensions. In either case, we can scale the floor area as the ratio of either capacity or number of units. Two hypothetical equations are:

$$A_{new} = A_{base} \left(\frac{N_{new}}{N_{base}}\right)$$

and

$$A_{new} = A_{base} \left(\frac{P_{new}}{P_{base}}\right)^{n}$$

where:

A_{new} = changed area of the generator building

A_{base} = area of the baseline generator building (from point design drawings)

N_{new} = number of small units in the changed design

N_{base} = number of small units in a baseline design

P_{new} = generator capacity in a changed design

P_{base} = generator capacity in a baseline design

n = an exponent relating generator floor size and generation capacity.

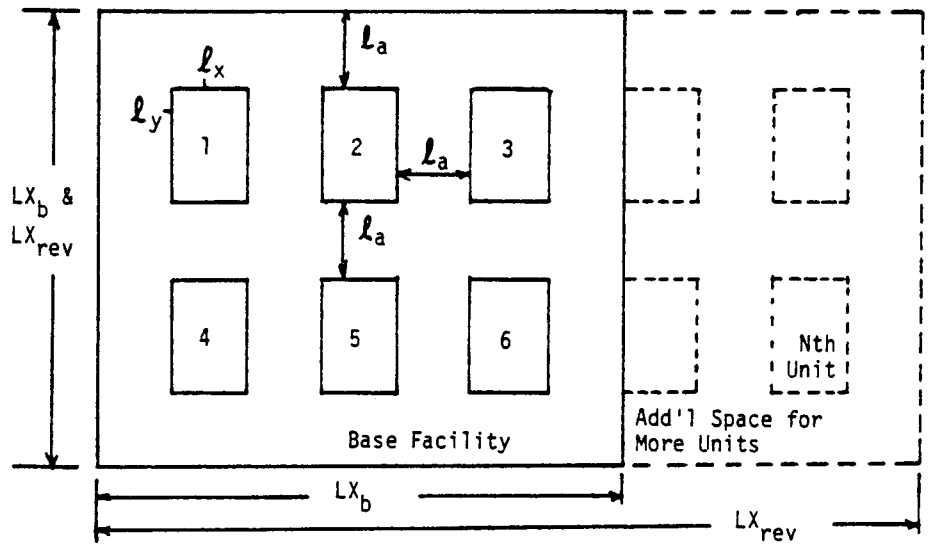
Figure 5.9, another simple example, illustrates the geometrical considerations in area scaling.

Once the various process areas have beev determined by such equations, they are totaled under the assumption that the sum of the various areas can be configured into a geometrically reasonable building.

Other Design Considerations

Other factors to be incorporated in the complete generated design are a preliminary estimate of site acreage and layout, energy and water consumption, and an estimate of the use of consumables other than energy.

The site layout model should estimate the floor areas of such auxiliary buildings as warehouses, office buildings, and switch houses as well as the overall site area. The process building area and material flow rates often constitute the parameters driving this part of the model.



- Each production unit occupies floor area $A_{unit} = (\ell_x \ell_y)$
- Baseline design requires six production units
- Aisle width ℓ_a assumed
- Baseline process building area represented by:

$$(A_{PB})_{base} = (LX_b)(LY_b) = (3\ell_x + 4\ell_a)(2\ell_y + 3\ell_a)$$

Suppose Performance/Design Modules Specify Additional Units for a Total of N Units:

$$(A_{PB})_{rev} = (LX_{rev})(LY_{rev})$$

$$= \left[\left(\frac{N}{2}\right)\ell_x + \left(\frac{N}{2} + 1\right)\ell_a\right](2\ell_y + 3\ell_a)$$

Figure 5.9

Sample Process Equipment Layout Model

The energy balance model should calculate the energy requirements for plant operation as a function of required hardware performance. This information is necessary to size the electrical switchyard and electrical distribution system, steam plant, fuel storage facilities, and process cooling requirements.

The above items represent the general considerations which must be addressed in conceptualizing the hardware-oriented portion of the process design model. It should be borne in mind that the computer, via the use of design algorithms, is really performing in a rudimentary manner, the effort of an entire design team, but in a lot less detail. The advantage is that the computer can redesign the process very quickly and compensate for the effects of off-baseline operating conditions, whereas each such effort would take a human design team several days at best.

The deviation/transfer function/response framework and its reoptimization capability requires a comprehensive knowledge of the process performance and design issues. For this reason there is no simple algorithm or specific procedure for building the performance and design models. The next chapter, which deals with the cost module, is less abstract and less process specific than the performance and design model.

CHAPTER VI

DEVELOPMENT OF COST MODELS

Purpose of Chapter

This chapter has as its purpose documentation of cost scaling techniques, i.e., calculation of the cost effects of a deviation in one or more elements of the input variable array, X. Most of the cost changes will be directly forced as a result of X_i driven changes in the internal variables, Q_i, i.e., design requirements passed from the design module. There are some external input variables, $(X_i)_{cost}$, however, which might be highly uncertain and enter directly into the economics calculations without first passing through the performance and design models. In the reactor example of Chapter V two such variables were the unit cost of feed and the unit cost of catalyst. For other processes such $(X_i)_{cost}$ variables might be unit power costs, scaling coefficients, reliability data and multipliers on the baseline unit cost of important process hardware items.

The user should attempt to model as many known costs as possible, striving for a uniform level of detail and impact across the several systems comprising the plant. The objective is to be inclusive; that is, to make sure that all elements which affect annual production costs are included in its calculation, even if the estimate for a given class of items is very rough. For this reason this chapter will include a discussion of reliability and cost estimating allowances in addition to the material on the scaling of capital and operating costs.

In Appendices F and G very generalized FORTRAN models for both capital and operating costs will be presented. These models are based on the principles discussed in this chapter. Appendix H contains an improved FORTRAN economic assessment code for the XYZ company example.

Plant Life Cycle

For this model only the two major elements of the plant life cycle, capital and operating costs, will be considered. Development costs and decommissioning costs are not included as part of the analysis.

The definitions of capital and operating costs differ somewhat between industries, textbooks, (such as Peters & Timmerhaus[70]), and cost estimating engineers. To some degree, the definitions arise from financial and accounting considerations. Appendix B contains a glossary of these terms as used in this document.

Capital costs are assumed to include the hardware and facilities required, including construction costs, prior to the time steady-state production is reached. Operating costs include the labor and material purchases necessary to maintain that production over the length of the production campaign and certain interest charges. The elements of each of these groupings will be discussed in more detail.

Before considering cost scaling in detail, it is now useful to discuss the concept of reliability and its effect on process economics.

Reliability Modeling

The overall subject of reliability is often abbreviated RAM (reliability-availability-maintainability) to simultaneously consider

its effects on a process. Both the capital and operating costs can be strongly affected by RAM considerations as shown in Figure 6.1. The relationships shown in Figure 6.1, such as number of spares, number of replacements, availability, etc., represent internal variables or Q_i values within the three-module transfer function model. Elements of RAM theory will eventually appear in all three modules, however, the majority of the RAM effects show up in the total annualized cost calculation rather than the productivity calculation, hence consideration of RAM in this chapter rather than the previous. Construction of a detailed RAM sub-module would usually occur after the baseline cost projection is complete and preliminary reliability estimates are available.

Reliability is a term applied to individual components or systems and represents the probability that over a given time, t, the component or system will not fail. In its most simple form, reliability can be expressed as a projected mean-time-between-failure (MTBF). The MTBF is also used to calculate process operating costs since its inverse roughly approximates the replacement rate for a particular item. If one knows the mean-time-to-restore (MTTR), i.e., repair or replace, an item, one can obtain the individual component availability as follows:

$$A = \frac{MTBF}{MTBF + MTTR}$$

where MTBF and MTTR are in the same time units. Uncertain MTBF and MTTR values for crucial process hardware often comprise input data, i.e., $(X_i)_{cost}$ variables to the model.

The availability of an overall plant or system can be calculated by breaking it down into its components via construction of a reliability

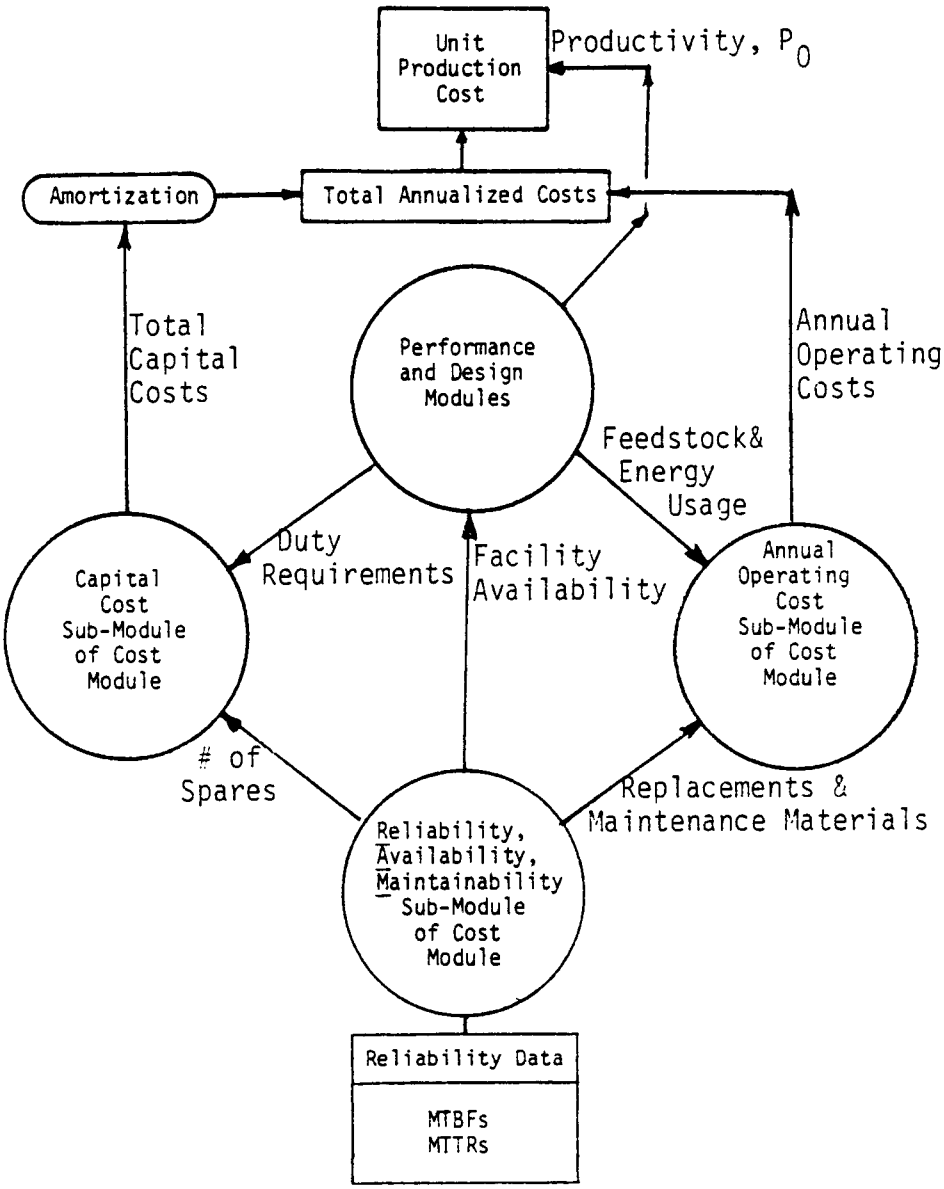


Figure 6.1

R.A.M. Interactions in Process Economics

logic diagram and application of the proper mathematical algorithms. This procedure is the subject of many excellent reliability texts. If the availability of particular plant items of interest changes in an off-baseline calculation, the calculated productivity of the plant will also be altered. If the estimated availability falls below the availability predicted for the baseline plant, the equipment capacities in the plant must be revised upward by the design module to compensate for the shortfall and have the plant still meet the desired productivity goal. In essence, this is a way of compensating for down time by adding parallel production units to the plant or resizing existing equipment. For this reason high productivity requires a high availability or plant on-stream fraction. Overestimates of plant availability in early cost and performance projections are very common. The consequences of this are considerable increases in plant size and capital costs in later estimates when a lower, more realistic value for plant availability has been identified.

Component reliability affects capital costs in other ways; the number of spare items for inclusion in the capital cost estimates depends on the number of items in the repair pipeline at a given time. If the time to actually repair (not just replace) an item is a significant fraction of its MTBF, spares must be initially purchased and be available for replacement of broken down items while the latter are being repaired. The number of spares is calculated as follows:

$$N_S = \frac{(N)(MTTR)}{MTBF}$$

where:

N_S = the number of spares

N = design number of units in the plant

MTTR = mean time to restore one unit

MTBF = mean time between unit failures.

To avoid production loss, spares must be available; if the MTTR value approaches that of the MTBF, the spares required may constitute a significant capital cost.

Major component MTBFs may heavily drive the annual replacement materials cost category of the operating costs. The annual replacement frequency, F_r, is calculated as follows:

$$F_r = \frac{N_r A}{MTBF}$$

where:

N_r = number of units in the plant

MTBF = mean time between unit failures

A = plant availability or on-stream fraction.

The short treatise on reliability above was included for the purpose of illustrating the interactiveness of the various components of the DTFR modeling system and the important role that reliability estimates play in assessing new processes where component reliability is likely to be an economic issue.

The Cost Scaling Models

The capital equipment duty requirements and replacement requirements generated by the process design model, for each set of input variables, X_i, are passed to the cost scaling economic model as Q_i values from the design model. The purpose of cost scaling is to properly reflect the

economic effects of design deviations from the baseline process. By design deviations are meant specifications changes, i.e., duty or capacity changes for particular equipment items which are dictated by the predecessor performance and design models. In the simple plug flow reactor example considered previously, one would be interested in how changing the reactor volume, V, would affect the capital cost of the reactor vessel itself.

Capital Costs: Identification of Cost Centers and Cost Drivers

Given a design alteration from baseline, one arrives at the revised capital costs by methods of cost scaling. Cost scaling consists of three important steps: (1) identification of an inclusive set of cost centers which cover all capital cost components; (2) identification of the key externally supplied $(X_i)_{cost}$ and internally generated Q_i variables capable of driving their cost; and (3) construction of mathematical algorithms, i.e., cost scaling equations, to relate each cost to one or more characteristics of the design, i.e., $C=C\ [Q_1,Q_2,Q_3,.,.,(X_i)_{cost}]$, where Q_1, Q_2, Q_3, etc., are the key design characteristics.

Cost centers are the accounting group into which particular hardware items are placed. For an economic evaluation in the early development stages, it is not necessary or advisable to have a cost scaling relation for every individual item project for the plant. Many items can be grouped; for example, the heat exchanger category can include all heat exchangers in the plant and represent a single cost center. For many applications the total cost for a cost center will be found to

scale with only one or two major plant operating requirements. For example, the cost of all the cooling towers in a gaseous diffusion plant can be directly scaled with the electrical power input to the plant.

The baseline design cost estimate provides a list of capital cost centers in the plant and aggregates individual costs into those centers. In a first engineering estimate, as might be performed for a RD&D Level II or III process, perhaps 10 to 50 capital cost centers will be used. Selection of capital and operating cost centers for scaling equation development is based primarily on the evaluator's and developer's knowledge of the process design and its principal driver variables and his or her feeling for which capital costs are most likely to change with design modification.

Each capital cost center has associated with it a total equipment cost which usually includes the purchase cost, delivery cost, installation labor and materials, checkout and start-up costs, indirect charges, and procurement costs. The cost center cost therefore represents the projected cost for equipment on the process floor, installed and ready for operation.

Key variables, whose values drive subsystem costs, must be identified. A few guidelines are available. For conventional chemical process equipment, geometric factors such as tower diameter, tower height, and tank volume constitute proper scaling variables. Variables related to the duty or mass or energy throughput of a component are also frequently used for both capital and operating cost scaling. For energy conversion processes, the heat duty or heat production rate may be the important capital cost driver. For electrical equipment, the installed

power capacity of the device may drive its capital cost. Buildings are usually costed on a per-square-foot or per-cubic-foot basis, hence the overall area calculated from the process layout will ultimately determine process building capital costs. The nature of these relationships is better understood when actual construction of the capital cost scaling equations is attempted.

Construction of Capital Cost Scaling Algorithms

It is usually sufficient to use one to four variables per cost equation. A single driving variable will often suffice. Cost ratioing with scaling exponents is a traditional, accepted method of cost scaling. For more detail see, for example, the articles by D. J. Chase[71] and A. Pikulik and H. Diaz[72] and such standard chemical engineering texts as Aries and Newton.[73] The new cost is generally calculated in the following manner:

$$C_{new} = C_{base} \left(\frac{Q1_{new}}{Q1_{base}}\right)^{Y} \left(\frac{Q2_{new}}{Q2_{base}}\right)^{U}$$

where:

C_{new} = the cost of the altered item

C_{base} = the baseline cost from the engineering estimate

Q_{new} = the value for the design attribute or driver after alteration from baseline

Q_{base} = the baseline value for the design attribute

Y,U = the capital cost scaling exponents.

The attribute Q may represent height, diameter, flow rate, volume, pumping head, duty, capacity, etc. For conventional process equipment

used in the chemical process and energy industries, values for scaling exponents are often available. Where significant economy of scale is present, the exponent will be significantly less than one. The "six-tenths" scaling rule is a familiar example. For first-of-a-kind hardware in the early development stage, scaling exponents are often not available.

Capital cost scaling is often handled by assigning a "dollars-per-unit attribute" to the hardware item and assuming linear scaling. Lasers, for example, are often discussed in terms of dollars-per-watt of photon output. If one knows the laser power requirements, then estimation of the total laser capital cost is merely a matter of multiplying this unit cost by the photon power requirement.

Learning Curves

For unique process hardware items which are to be purchased in quantity, the number of items required may affect the cost of each. This "learning curve" effect results from the fact that improved manufacturing techniques and operating experience lower the unit cost of production for these items as time proceeds. A good example of a process where learning plays an important role is the gas centrifuge process for which thousands of centrifuge machines must be manufactured and installed in a plant.

The learning rate fraction R_ℓ represents the fixed ratio of the unit cost of producing a second unit (or lot of n objects) to the cost of producing the first unit (or lot of the same size n). If the cost of a first lot or unit is C_1, the cost of the mth lot or mth unit will be:

$$C_m = (C_1)m^G$$

where:

$$G = \frac{\ell n(R_\ell)}{\ell n\ 2}$$

and R_ℓ is the learning rate fraction.

For example: For a 90% learning curve, $R_\ell = 0.9$. The unit cost for the second lot, C_2, i.e., for m = 2, would be $2^G(C_1)$, where G = -0.1515, or 0.9 times the cost of the first lot.

Learning curve theory is especially useful and important in pioneer process situations, especially those in RD&D Level IV, where a development item necessary to the process is first entering the manufacturing stage, and it provides the cost estimator a convenient means of quantity scaling. The Set III gas centrifuges for the enrichment of uranium now being manufactured and installed at GCEP are a good process equipment example.

Calculation of Direct Costs

In this chapter the intent is not to consider accounting and scaling procedures for all types of process equipment or facilities, but rather to discuss the modes of thinking required. Once the capital cost scaling algorithms are constructed they should be programmed and tested by submitting the baseline operating and design variables to the cost code. The resulting capital costs for each cost center and the total should closely approximate the cost figures in the detailed baseline estimate which was prepared with the assistance of engineering estimators. The sum of all special process equipment, auxiliary and support items, including process start-up and spares, constitutes the total of

the direct capital costs. Table 6.1 shows typical cost centers which might occur in each category. By special process equipment is meant that which is exclusive to the application of interest. The remaining equipment, much of which is typical auxiliary or support equipment found in any process or power plant, is often referred to as the balance of plant or simply "BOP."

To complete the capital cost model, indirect capital costs must be added to cover engineering, contingency, and, since the discounted cash flow method (i.e., the time phasing and discounting of capital expenditures) is not being used, interest during construction must be added. Each indirect cost is discussed separately below.

Engineering Costs

For first-of-a-kind or immature projects, engineering manpower costs can represent a considerable fraction of the direct capital costs as compared to processes reduced to practice. Several factors contribute to these higher engineering costs:

1. Whereas most conventional equipment can be designed and costed from "handbook" or in-house historical data, this is not the case for first-of-a-kind technologies.

2. The engineering team must learn a new technology and, in cooperation with the development team, devise new design procedures.

3. Obtaining capital cost information on crucial new-technology items often requires vendor studies, i.e., engineering and economic feasibility studies performed by the potential suppliers of these items.

4. Unforeseen process integration problems and the frequency of mandated changes often require redesign of particular systems. The

Table 6.1

Typical Cost Centers Constituting
Capital Costs

Special Process Equipment
(Process-specific)
Process Auxiliaries
Piping and valves
Transformers
Heat exchangers
Instrumentation and controls
Pumps and compressors
Process Buildings
Process Support
Cooling towers
Electrical distribution and switchyard
Steam plant
Waste disposal
Fencing and security
Shops
Site Costs
Land acquisition
Site preparation
Indirects
Engineering
Contingency
Interest during construction

final detailed engineering design and cost estimate for a plant may bear little resemblance to the first or second less detailed estimates performed at earlier RD&D levels.

The engineering cost for early estimates is generally calculated as a fraction of the direct costs and is most often projected by the design engineering team. Typical values for immature processes range from 20% to 40% of indirect costs. The higher the percentage of new technology in a proposed process, the greater will be the engineering allowance.

Contingency

Contingency is an allowance used to adjust a capital or operating cost estimate based on an incomplete design so that it accurately reflects current experience. For early estimates, it is typically large because of the limited design detail available to the cost estimator. Contingency is often misinterpreted as a catch-all adjustment factor to cover all causes of capital cost underestimation and performance overestimation. Its correct definition does not include the latter, and its incorrect determination is a partial cause of the former. Capital cost contingency is related to the engineer's assessment of the completeness and inclusiveness of the capital cost estimate for various cost centers. Although experienced estimators can sometimes assign a contingency allowance to the project as a whole, as more detailed estimates are generated the overall contingency should be calculated by weighting the contingency allowance for each cost center by the fraction of the capital cost arising from that cost center and summing the products.

If a cost center consists of conventional equipment items with which the engineering staff has design and cost experience, the

contingency for this cost center will be low, perhaps as low as 15%. For newly developed hardware to be used in a process for the first time, a higher contingency, usually anywhere from 40% to 100%, is assigned. In early engineering estimates, 20% to 40% is used for buildings and conventional equipment, such as cooling towers, electrical switchyards, and electrical distribution systems. The engineer is essentially saying that with new technology he or she needs to include a significant percentage for possible hardware items omitted, possible equipment installation difficulties, and possible equipment and testing problems.

Contingency should not be applied to the process as a whole; rather, it should be the sum of many separate contingency determinations. It should not consider attributes such as overall process complexity, performance degradation, susceptibility to environmental and sociopolitical problems, and reliability shortfalls. The uncertainty analysis techniques and models can be used to calculate the effects of some of these factors.

Whether a process technology is new or not, if one gives an engineering design team fabrication quality drawings, a highly accurate cost estimate is likely to be returned. If built according to the drawings, however, the device still may fail completely or not meet the performance specifications needed to achieve the desired productivity. This fact is mentioned to underscore the fact that contingency is not a measure of possible productivity shortfalls.

Interest During Construction (IDC)

This cost category accounts for the interest expense on funds borrowed to pay the bills for materials (including process equipment)

and labor (including engineering) used during construction. Essentially the IDC is the cost of plant the construction loan. Since early estimates often do not include the generation of a capital investment spending pattern, the calculation of the IDC multiplier can be made by assuming a generalized spending pattern. The simplest case would be to take the sum of the direct capital cost, engineering, and contingency, and divide the sum by the projected project construction time. One can then calculate the future worth of this series of uniform payments as follows:

$$C_{ST} = C_D + C_E + C_C \quad \text{and} \quad C_{AN} = \frac{C_{ST}}{n}$$

where:

C_D = direct capital cost

C_E = engineering cost

C_C = contingency cost

n = years for construction

$$F = C_{AN}(1+i)^n + \frac{C_{AN}(1+i)^{n-1} - 1}{i}$$

where i = interest rate and F = future worth.

The interest paid over the n years would be $F - C_{ST}$ and the IDC fraction would be $(F - C_{ST})/C_{ST}$.

In most projects, the spending over the construction period is not uniform, but rather the cumulative pattern is in the shape of an S-curve. The analogous future worth calculation is more difficult since separate terms are involved for each year; however, the result is more realistic. Multiplication of the uniform spending pattern IDC fraction by a shape

factor of 0.7 will give a good approximation to an S-curve spending pattern IDC. A paper by D. L. Phung[74] discusses the calculation of IDC for various spending patterns.

Total Capital Cost

The total capital cost, sometimes also referred to as the TEC or total estimated cost, is the sum of the direct and indirect (engineering, contingency, and IDC) costs. Since capital money is spent early in the total life cycle of a project, it is often an important figure of merit for planners and budgeters. Amortization or recovery of these capital costs and their inclusion in the total annualized costs is discussed in the next few paragraphs on operating cost scaling.

Operating Costs: Identification of Cost Centers and Cost Drivers

The annual operating costs consist of essentially five annual cost centers: labor, materials, utility usage, interest on inventories, and interest on working capital. Early in a development project there is generally very little available data on predicted operating costs except for perhaps preliminary estimates of feed costs, utility consumption and costs, and a few reliability estimates for key replaceables. The methodology for obtaining more detailed operating cost data is described below, along with operating cost scaling guidelines.

Labor Costs

Until a pilot plant or demonstration plant is constructed for the new process and some operating experience is gained, satisfactory work force size determinations for a large-scale facility can be best approached through operations analysis, i.e., the division of plant

operations into human-performed functions and design of a logistics system to support them. The five functional categories of administration, plant operations, plant maintenance, component refurbishment, and plant support serve as a starting point for an operations analysis study. In larger facilities the functional staffing categories above can be further subdivided into four personnel categories: managerial/professional, clerical, technical support, and craft labor (e.g., process operators, maintenance mechanics, and material handlers for the latter). The analyst's next task is to define the procedures necessary to operate the plant and calculate the time and material requirement for each task, the level of expertise, and job description for each. When tasks must be performed around-the-clock, shift operations are required.

To illustrate the chain of thought the analyst might follow, consider a process in which hundreds of filter beds must be changed each day. The time necessary to change one bed allows calculation of the man-hour requirement for this activity. In converting man-hour work content to a staffing estimate, one must take into account rest breaks, vacation time, sick leave, and other time not worked. From the man-hour work content, work requirements, and number of shifts, a total number of laborers for this category can be determined. For many administrative and support tasks, such as supervisor and maintenance technician, the staffing can often be calculated as a fraction of the total craft labor staff.

Labor requirements are closely related to equipment reliability and performance assumptions. The lifetime or MTBF of a component determines its replacement frequency, hence it also defines the replacement labor. If a process consists of parallel units, the deviation from baseline productivity will change the number of units, hence changing the number of operation and maintenance personnel required on the process floor.

In a FORTRAN computer code the staffing estimate is easily handled by an accounting system utilizing doubly dimensioned arrays in which personnel salary category and functional categories constitute the two dimensions. Rules for truncation and rounding must also be devised to prevent the calculation of fractional persons in the labor scaling equations. The labor cost is calculated by multiplication of the staffing person count array by the salary array. Fringe benefits are added as a percentage of direct labor costs, usually on the order of 20% to 40%.

As with capital costing, a contingency allowance is needed to account for the lack of detailed process definition. Early estimates for staffing tend to overlook some unforeseen tasks which for later actual plant operation must be staffed. The operations analyst may choose to add a contingency allowance to the total staffing cost in order to adjust for this shortcoming. For a process at RD&D Levels I through III, a 20% or greater contingency would be appropriate.

Materials Costs

Three general categories of operating materials can be identified for modeling: Feedstocks or raw materials; replacements for failed or worn components, and work materials.

Feedstocks, representing the raw materials needed for production, are often a significant fraction of the operating cost of a facility. Examples would be the coal purchased for a gasifier, enriched uranium purchased for a nuclear power plant, and deuterium-tritium fuel for a fusion power plant. Other items which are purchased consumables might be reagents, catalysts, lubricants, coatings, or adhesives required for a particular manufacturing process. The consumption and costs of these materials can be calculated from computer-generated material and energy balances, which give annual average rates of use, and these balances are available from the performance and design modules. Unit costs for materials are often uncertain inputs to the cost model.

Replacement materials requirements are calculated from the reliability model as was discussed in an earlier paragraph. The unit costs for replacement items are often subject to uncertainty, hence the unit cost of a replacement item and its estimated lifetime are often input variables, $(X_i)_{cost}$, of interest.

Work materials include expendable tools, cleaning compounds, clothing, and office supplies used by the staff in performance of plant operations. Their usage rates can be calculated as a fraction of labor cost. The estimator should also add a contingency to the total materials cost to cover materials not defined in the baseline but which are likely to be needed in an actual production facility.

Utility Costs

Utilities represent consumables which supply work, heat, cooling, etc., and are not actually physical parts of the commodity being produced. Examples are electric power, high pressure steam, sanitary

water, process water, sewage treatment, and compressed air. Unit utility costs are usually well known and are quoted in the form of dollars per kilowatt-hour, dollars per thousand pounds of 600 psia steam, dollars per 1000 gallons of water, etc. The difficult part of the analysis is determination of utility consumption. Energy balances and the process design code supply much of the necessary data; however, one must adjust for the process availability and energy losses. The former is important since the operating electrical load of the plant at any time must remain below the design or nameplate electrical capacity of the switchyard equipment. In the calculation of electrical power usage, power factors and efficiences are used to back-calculate the total switchyard load from the energy consumed in the process in the forms of heat, work, or lighting, etc. Electrical or steam requirements for heating and ventilating depend on building area or volume. Process water requirements depend on heat exchange requirements for process cooling. Sanitary water and sewage treatment requirements generally scale with the staff size. If the above costs are available from the detailed estimate for the baseline process, off-baseline costs can be calculated by simply ratioing the use rates for each utility category, i.e.,

$$C_{new} = \left(\frac{U_{new}}{U_{base}} \right) C_{baseline}$$

where U represents annual usage and C an annual utility cost.

Inventory Costs

To ensure continuous operation of a plant it is necessary to maintain an in-process inventory of spare parts or critical operating

materials. This represents money tied up in inventories and is considered an investment. In a chemical plant the various process holdups constitute an important inventory. The inventory charge is calculated by multiplication of the assumed interest rate by the levelized annual amount of inventory.

Interest on Working Capital

The working capital represents the cash on hand to cover current costs of labor, materials (including feedstocks but not holdups or spares included in the inventory costs category above), and utilities. Since this working capital must be maintained, an interest charge is accrued to it. One current estimating practice is to set the working capital requirement at two months' worth of the charges to these categories. Then the interest on working capital is given by

$$C_{IOWC} = \left(\frac{2}{12}\right) (i) (C_{LAB} + C_{MATL} + C_{UTIL}) ,$$

where:

C_{IOWC} = the charge for interest on working capital,

C_{LAB} = annual labor cost (including fringes and contingencies),

C_{MATL} = annual material costs (including contingency),

C_{UTIL} = annual utility costs, and

i = the annual interest or discount rate.

Total Annualized Cost Calculation: Amortization Portion

Recovery of the total capital investment is handled by using the capital recovery factor, which is the inverse of the uniform series present worth factor:

$$CRF = \left(\frac{A}{C_{CAP}}\right) = \frac{i}{[1-(1+i)^{-n}]} ,$$

where:

i = annual interest rate,

n = number of years to amortize project,

A = annual payment to amortize,

C_{CAP} = total capital cost, and

CRF = capital recovery factor.

The CRF converts the total capital cost into a levelized payment which recovers the investment over n years and allows the investor a return of investment at 100i% per annum on the unrecovered capital. For government energy projects, the presently preferred (FY 1984) inflation free discount rate and amortization period are 5% and 25 years, or a CRF of 7.09%.

Total Annualized Cost and Unit Production Cost Calculation

The total annualized cost is the sum of the annual operating costs and the recovered capital cost discussed above:

$$C_A = C_{LAB} + C_{MATL} + C_{UTIL} + C_{INV} + C_{IOWC} + (CRF)C_{CAP} .$$

The unit production cost is the quotient of this total annualized cost cost and the average annual production rate or productivity P:

$$C_{UNIT} = C_A/P .$$

Testing the Models

Having productivity, design, and production cost models available, the next test is to check whether utilizing the baseline input variables will regenerate the same calculated design parameters and production

cost breakdown as found in the original baseline design and cost estimate made before the model was constructed. Once such consistency is demonstrated, key input variables can be varied one-at-a time utilizing single variable sensitivity studies to determine whether the figures of merit calculated behave in a logical manner with respect to individual variables. For example, if one increases an electrical efficiency term, the predicted power use, utility costs, and total operating costs should decrease. As will be discussed in a later subsection, single variable sensitivity studies can also be used to identify key production cost and productivity driving variables which will later become uncertainty analysis inputs. If the model passes the above tests, one can be reasonably certain that off-baseline cases involving deviations in many inputs will be handled in a physically and economically reasonable manner.

Example Cost Scaling Models

For purposes of illustration, a typical very short FORTRAN capital and operating cost model has been constructed which incorporates many of the economic principles discussed previously. Table 6.2 shows a sample output table typical of FORTRAN coding for the capital costs contained in Appendix F. Table 6.3 is a sample output table from a hypothetical operating cost model contained in Appendix G. For brevity the output formatting coding has been omitted from some of these FORTRAN listings.

These models as shown cannot be applied to any new process; however, they are very typical of what is required in process assessment. The user, based on his experience, knowledge, and baseline

Table 6.2

Typical Output Table from
Capital Cost Scaling Model

* * * PLANT CAPITAL COST ESTIMATE * *	THOUSANDS OF $
SPECIAL EQUIPMENT ITEM 1	30000.0
SPECIAL EQUIPMENT ITEM 2	22000.0
12 UNITS OF SPECIAL EQPT ITEM 3	500.0
ITEM 3 SPARE UNITS	125.0
TOTAL SPECIAL EQUIPMENT COST	52625.0
COMPRESSOR	500.0
GENERATOR	750.0
REFRIGERATION	300.0
HEAT EXCHRS	100.0
PIPING	50.0
STORAGE TANK	30.0
PUMPS	70.0
RECIRC. WATER SYSTEM & COOLING TOWERS	800.0
OUTSIDE UTILITIES(INCL. SWITCHGEAR)	850.0
ELECTRICAL DISTRIBUTION SYSTEM	550.0
INSTRUMENTATION AND CONTROL	250.0
PRE-OPERATIONAL CHECKOUT& STARTUP	100.0
SPECIAL SHOPS	40.0
BUILDING	600.0
SITE	100.0
BOP SUBTOTAL	5090.0
TOTAL DIRECT COSTS	57715.0
ENGINEERING AT 30.000 % OF DIRECT COSTS	17314.5
SUBTOTAL	75029.5
CONTINGENCY AT 35.000 % OF ABOVE	26260.3
SUBTOTAL	101289.8
INTEREST DURING CONSTRUCTION AT 18.000 %	18232.2
TOTAL CAPITAL COST	119522.0

Table 6.3

Typical Output Table from Operating Cost Scaling Model

* * * TOTAL ANNUAL OPERATING COSTS IN THOUSANDS OF DOLLARS * * *		
LABOR COSTS:		
TOTAL DIRECT LABOR COSTS FOR A STAFF OF 686	13034.0	
FRINGE BENEFITS AT 35.0 %	4561.9	
SUBTOTAL	17595.9	
CONTINGENCY AT 20.0 %	3519.2	
TOTAL LABOR COSTS:		21115.1
REPLACEMENT & MATERIAL COSTS:		
.3E+08 UNITS O F FEED @ $ 0.050 @	1500.0	
48 UNITS OF ITEM 3 @ $ 41670. @	2000.2	
ADDITIONAL WORK MATLS	1231.7	
TOTAL REPLAC.& MATERIALS COSTS		4731.9
CONTINGENCY AT 20%	946.4	
TOTAL EXPENDABLES COST:		5678.2
UTILITY COSTS:		
4400.KW ELECTRIC POWER AT 0.04 PER KW-HR	1541.8	
STEAM	290.0	
COOLING WATER	1.0	
OTHER UTILITIES	240.0	
TOTAL UTILITY COST		2072.8
INTEREST ON WORKING CAPITAL		481.1
INTEREST ON INVENTORIES		6.7
SUBTOTAL ANNUAL COSTS		29353.9
AMORTIZATION OF CAPITAL ($ 119520000. AT CAPITAL RECOVERY OF 0.1102) I.E. 10.0% INTEREST OVER 25 YRS:		13167.3
TOTAL ANNUAL COSTS		42521.2
UNIT COST FOR PRODUCTIVITY OF .25E+09 UNITS/YR:	0.170	

cost estimate, must supply the actual algorithms. Many of the cost centers and algorithmic forms shown, however, are likely to appear in the users application. In the capital cost model (Appendix F), cost centers along with appropriate driver variables are given in the form C (cost center) = F (cost driver Q_1, cost driver Q_2). The user can supply his or her own actual functional form by a combination of intuition, design knowledge, and use of the single cost data point supplied by the cost estimator upon which the functional form can be "pivoted". The functional forms shown in Appendix F are illustrative examples.

In many cases certain cost centers can be omitted. For a solar power plant, for example, one would not need a process building or a refrigeration system. It is more important, however, to examine the proposed process closely to determine which cost centers are, rather than are not, to be included. The two sample FORTRAN models in Appendix F and G should give the user a starting point from which to begin development of cost scaling algorithms.

The cost center designated "special process equipment" includes the novel and process-specific items that usually form the heart of the process. In the examples in Table 6.2 and Appendix F, three fictitious items are scaled in this cost center. They do not represent real equipment items, but rather different types of scaling relationships. The cost of item 1 is assumed to scale exponentially with two internal variables, the cost of item 2 scales with a unit hardware cost input, and item 3 represents a replicated item for which spares and replacements must be provided. These three generic items were chosen mainly to

illustrate the cost scaling and reliability principles discussed previously.

These example cost scaling models are very simple and the reader might at first consider them unrealistic. For an actual process evaluation application, however, the models will grow rapidly and become significantly more detailed and be better validated by subsequent cost estimates. Fifty or more cost scaling algorithms for a process would not be unusual. The photochemical process analysis described in Appendix I and the FORTRAN assessment code listing for it (Appendix J) should give the reader a feeling as to the complexity involved.

Algorithms for the XYZ Catalyst Example

With the preceding cost scaling principles and the optimized reference design variables from Chapter V, one can construct an improved model for the catalyst problem described in Chapter V. Appendix H contains the FORTRAN coding for the entire XYZ assessment model, including performance, design, and cost scaling relationships. Table 6.4 shows the new optimized baseline design and unit cost which can be derived from this model. It is assumed that the cost scaling algorithms were developed from data generated by cost estimators, thus they represent an improvement over the original cost-scaling algorithms in Chapter V and Appendix E which were utilized to obtain the optimized development reference design.

This same XYZ process assessment model will be utilized as the example model for illustrating the use of the Monte Carlo technique in Chapters XIII and IX.

Table 6.4

Optimized Baseline Design
and Costs for XYZ Process

SUMMARY OF INPUT DATA
CA0 = 0.100
DCAT = 5000.
K = 96.0
P0 = 2800.

K = 96. CF0 = 0.050 CCAT = 1.00

OPTIMUM CASE

CA0 = 0.100
DCAT = 5000.
K = 96.0
P0 = 2800.

I = 64 XA0 = 0.64 FA0 = 1093.8 V = 246.8 CUNIT = 0.0858
* * * PLANT CAPITAL COST ESTIMATE * * THOUSANDS OF $

SPECIAL EQUIPMENT ITEM 1(REACTOR)	138.2
SPECIAL EQUIPMENT ITEM 2(CATALYST)	1234.2
SPECIAL EQPT ITEM 3(SEPARATOR)	31.9
TOTAL SPECIAL EQUIPMENT COST	1404.4
COMPRESSOR	16.4
HEAT EXCHRS	2.2
PIPING	6.6
STORAGE TANK	21.1
OUTSIDE UTILITIES(INCL. SWITCHGEAR)	90.0
ELECTRICAL DISTRIBUTION SYSTEM	70.0
INSTRUMENTATION AND CONTROL	10.0
PRE-OPERATIONAL CHECKOUT& STARTUP	50.0
BUILDING	453.6
SITE	10.0
BOP SUBTOTAL	729.9
TOTAL DIRECT COSTS	2134.2
ENGINEERING AT 30.000 % OF DIRECT COSTS	640.3
SUBTOTAL	2774.5
CONTINGENCY AT 32.000 % OF ABOVE	887.8
SUBTOTAL	3662.4
INTEREST DURING CONSTRUCTION AT 18.000 %	659.2
TOTAL CAPITAL COST	4321.6

Table 6.4 (Continued)

* * * TOTAL ANNUAL OPERATING COSTS IN THOUSANDS OF DOLLARS * * *

LABOR COSTS:		
TOTAL DIRECT LABOR COSTS FOR A STAFF OF 18	342.0	
FRINGE BENEFITS AT 35.0 %	119.7	
SUBTOTAL	461.7	
CONTINGENCY AT 20.0 %	92.3	
TOTAL LABOR COSTS:		554.0
REPLACEMENT & MATERIAL COSTS:		
.1E+08 UNITS O F FEED @ $ 0.050 @	479.1	
ADDITIONAL WORK MATLS	32.3	
TOTAL REPLAC.& MATERIALS COSTS		511.4
CONTINGENCY AT 20%	102.3	
TOTAL EXPENDABLES COST:		613.7
UTILITY COSTS:		
481.KW ELECTRIC POWER AT 0.04 PER KW-HR	168.6	
OTHER UTILITIES	40.0	
TOTAL UTILITY COST		208.6
INTEREST ON WORKING CAPITAL		22.9
INTEREST ON INVENTORIES		0.6
SUBTOTAL ANNUAL COSTS		1399.8
AMORTIZATION OF CAPITAL		
($ 4321599. AT CAPITAL RECOVERY OF 0.1627)		703.3
I.E. 10.0% INTEREST OVER 10 YRS:		
TOTAL ANNUAL COSTS		2103.2

The next chapter deals with the use of adjustment terms to four important components of the unit production cost for the purpose of improving very early (RD&D Level I) estimates. Such an attempt allows one to compensate for modeling deficiencies in the earliest evaluation efforts.

CHAPTER VII

THE USE OF CORRECTION FACTORS IN EARLY PROCESS MODELS

Deficiencies of Early Models

Although the previous two chapters have described in some detail the construction of an overall process and economic model, the analyst must still confront the fact that his models are incomplete and that a model developed very early in the RD&D program cannot include all causal phenomena or links between performance and economics which will eventually be identified as process development proceeds. The way in which this problem manifests itself is that pertinent information needed for the overall model, such as individual modeling elements discussed in the previous two chapters, is only partially available. Early "best guess" estimates and models constructed prior to the first engineering point design (i.e., in RD&D Level I) often fall in this category. These early evaluations may lack important modeling elements such as RAM or staffing algorithms.

The Introduction of Correction Factors at Various Levels of Detail

In early models, the analyst may wish to introduce correction factors into the models to compensate for the modeling deficiencies mentioned above. At the detail level such factors usually represent multipliers applied to internally generated figures of merit which quantify the performance of a poorly understood process step or phenomenon. Factors can also be applied to global economic figures of merit, such as

productivity, capital cost, and operating cost. As the models improve in quality and detail the use of correction factors tends to proceed toward the adjustment of detailed phenomena within a model as opposed to adjustment of global variables. If all phenomena affecting process performance and economics were understood, of course, no correction factors would be needed at all. The following paragraphs describe particular applications where the use of correction factors in early models would be considered legitimate.

Application to Unmodeled Phenomena

Modeling correction variables are multipliers used to allow for some degradation in particular productivity-related phenomena for which no detailed model exists, but for which it is known that an unexplained deleterious effect is present. Wherever possible, the use of these modeling correction variables in the productivity model is superior to trying to incorporate such uncertainties into a multiplier on a global figure of merit such as productivity. By applying them to the particular productivity determining phenomenon which they actually influence, the productivity effect is more correctly weighted than it would be if a multiplier on the productivity P_O were used to handle its effect.

As an example, suppose an electrical field is postulated to completely permeate a plasma in a fusion device. Plasma physicists know that 100% penetration of a plasma normally does not occur and that myriad contributing, unmodeled and in some cases unexplained effects may be causing this incomplete penetration behavior. If a particular productivity determining parameter depends on the average strength of a field

within a plasma, the analyst may allow for degradation effects by applying a fractional correction variable or multiplier that quantitatively gauges the effects of partial field penetration.

Application to Global Process Figures of Merit

The Rand pioneer plants study[75] suggests that factors modifying or adjusting the global process figures of merit might be a useful method of compensating for lack of knowledge in various process areas. The Rand study suggested two such factors, a cost growth factor to adjust capital costs and a performance discount factor to adjust productivity. Since these particular factors, as derived by Rand, are appliable only for a certain class of processes in later RD&D stages, the use of the Rand algorithms per se is discouraged as part of this evaluation effort. The concept of using correction factors with similar names and functions, however, may have some validity for early models. Four correction factors are here suggested and their overall effects impact the calculation of the unit product cost. Two of them, the performance discount factor, F_{PD}, and the capital cost growth factor, F_{CCG}, take their names from the RAND study and perform similar, but not identical, functions. The third, the operating cost growth factor, allows consideration of operating costs not covered in the models. The fourth--the project delay penalty factor, F_{PDP}--is an attempt to assess the cost consequences of construction delays not included in calculation of the interest during construction. The following equation, which sums the major components of the unit cost, shows how the four factors are used as multipliers on the appropriate components:

$$C_{UNIT} = \frac{(F_{CCG})[\{C_{DIR}+C_{ENG}+C_{CONT}+C_{IDC}(F_{PDP})\}(CR)+(F_{OCG})(C_{OPER})]}{P(F_{PD})}$$

where:

C_{UNIT} = the unit cost,

F_{CCG} = the capital cost growth multiplier,

F_{OCG} = the operating cost growth multiplier,

C_{DIR} = the direct capital cost,

C_{ENG} = engineering costs,

C_{CONT} = contingency allowance,

C_{IDC} = interest during construction,

F_{PDP} = project delay penalty factor,

CR = capital recovery factor,

C_{OPER} = annual operating costs,

P = annual production rate (availability corrected), and

F_{PD} = performance discount factor.

If the models were perfect there would be no need for such factors and the value of each would be unity. In most cases, however, the multipliers would have the following boundaries:

Performance Discount: $0.2 < F_{PD} < 1.2$

Capital Cost Growth: $10 > F_{CCG} > 0.8$

Operating Cost Growth: $10 > F_{OCG} > 0.8$

Project Delay Penalty: $5 > F_{PDP} > 1.0$

In a later subsection it will be seen that a range of values can be assigned to each via a probability density function. In many cases, especially those dealing with infant technologies such as fusion

energy, one of the endpoints will be unity, i.e., the case where the process performs and incurs costs as predicted by the model. The function of the four correction factors would be as follows:

(1.) Performance Discount (F_{PD}) - account for major deficiencies in the performance models, such as lack of reliability or availability effects on production. Other deficiencies would be the lack of understanding of crucial process phenomena.

(2.) Capital Cost Growth (F_{CCG}) - account for major deficiencies in the capital cost model, such as lack of cost scaling algorithms for balance-of-plant items or the non-application of estimating allowances.

(3.) Operating Cost Growth (F_{OCG}) - account for major deficiencies in the operating cost model, such as lack of reliability, staffing, or utility use algorithms.

(4.) Project Delay Penalty (F_{PDP}) - accounts for the possibility that the construction time for the project may be underestimated.

The two factors F_{CCG} and F_{OCG} might be useful under circumstances where no reference design for the process is available from a cost estimating engineer. The implication in this chapter is that for most processes the model itself is a very optimistic representation of the process. The problem at hand for the analyst is the determination of the pessimistic (high production cost, construction delay, degraded productivity) endpoints for F_{PD}, F_{CCG}, F_{OCG}, and F_{PDP}, i.e., the points farthest from unity. The more comprehensive and realistic the process model, the closer these "pessimistic" endpoints will be to unity. This is the same as saying that the more sophisticated the process model

becomes, the less weight need be carried by correction or adjustment factors.

Determination of Correction Factors

Selection of numerical values for these factors depends greatly on the intuition of the analysts and upon the state of the particular process model. For these reasons no attempt will be made to present algorithms or criteria for this determination. The best the analyst can do is to determine whether his or her models cover the various elements described in the previous two chapters. A typical mode of thinking might be following: "I know my first capital cost scaling model includes only the new process specific equipment and leaves out balance of plant items. I will add 30% (F_{CCG} = 1.3) to the capital costs to account for this deficiency."

As will be seen in the next chapter, uncertainties in these factors can be handled via the Monte Carlo method of multi-variable sensitivity analysis. The models can thus include and utilize ranges on these factors in performing an overall uncertainty analysis.

Some Cautions Regarding the Use of Factors

The only time the use of any such post-hoc factors is excusable is very early in the R&D stage when (1) cause-effect models are so primitive and imprecise that aggregation of effects is necessary or (2) values for major inputs are poorly known and their ranges are at best rough.

As the modeling effort proceeds in parallel with development, the analyst should eventually eliminate the use of such factors, since they reconvolve the very things he is trying to unravel--accumulation and propagation of uncertainty through causal links.

The use of these factors has been omitted from both the XYZ catalyst example. For the photochemistry process in Appendix I, an example of the simultaneous use of F_{CCG} and F_{PD} is shown for illustrative purposes only.

CHAPTER VIII

THE EVALUATION OF UNCERTAINTY

A Two Part Approach

With a process performance and cost model available, the emphasis of this technique will shift toward uncertainty analysis. The evaluation of uncertainty will be divided into two parts: (1) quantitative determination of the input variables and their ranges, and (2) application of the Monte Carlo technique.

The first item is the real assessment task and requires the gathering of data and the making of educated judgments thereupon. The second task represents the more straightforward application of a mathematical formalism; however, certain cautions are necessary and will be discussed.

The first step requires the user to closely examine and test the model and consider possible probability distribution forms for the key inputs to the model. These two procedures are now considered.

Determination of Uncertain Input Variables and Their Probability Distributions

Nature of Model Inputs

During the initial effort required to set forth a reference technology description and facility design suitable for cost estimation, the qualitative nature of a few of the key process input variables, X_i, to be considered becomes readily apparent. As subsequent models increase in complexity, however, numerous other input variables, X_i, may be added

by the analyst, and eventually he or she must sort out for uncertainty analysis the ones which are major determinants of process merit.

The single value sensitivity study (or SVSS) technique is the most useful method for sorting out, one-at-a-time, the input variables with the most unit cost impact. This method is most reliable when a variable is incremented closely around that input value which defines the reference base case. As a single value X_i deviates further from the base case, its range and figure-of-merit (Y) derivative, $\partial Y/\partial X_i$, may be misleading. In a complex multivariable model, even when other inputs $X_j \neq X_i$ are held constant as is the case for a SVSS, the reoptimization mechanism within the model may have readjusted the internal design parameters to ameliorate any adverse cost or productivity consequences of X_i being far from baseline. When in the multivariable sensitivity study (MVSS) mode, however, the model can do a much better job of optimizing since the overall constraints on the process are fewer. For this reason, SVSS results often tend to overstate a dependency of a figure of merit (such as unit cost) Y on a particular input value X_i.

Figure 8.1 shows an SVSS plot for several single variables, X_i, plotted on the same scale and with limited variable ranges. This type of plot allows selection of the important driver variables by means of indicating those with the greatest slopes $|dY/dX_i|$, where $\tilde{Y}$ and $\tilde{X}_i$ represent functional deviations in X_i and Y from their reference or base values.

Classes of Variables

To ensure consistency in application of this methodology to alternative processes, it is important that a systematic method be used to determine input probability distributions and values. Ideally one would

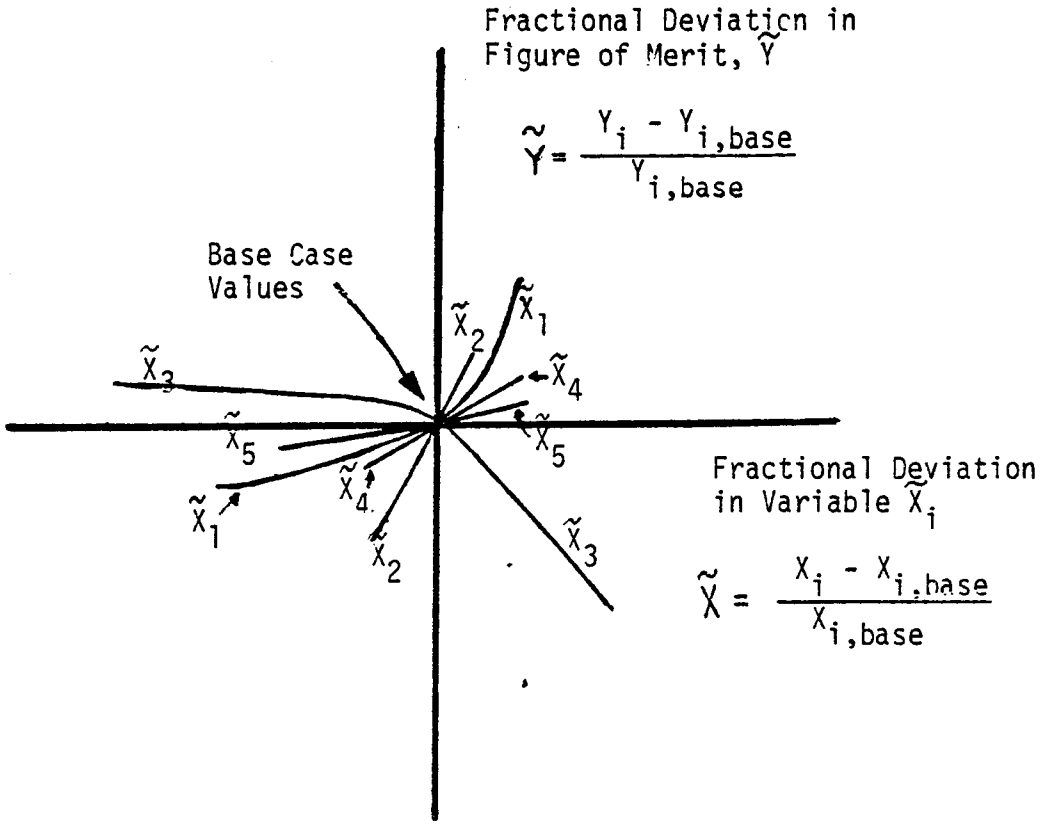


Figure 8.1

Sample SVSS Plots for Five Input Variables

prefer input values directly available from laboratory or larger scale experiments. A difficulty lies in the fact that often measurements of critical process variables are taken on subscale apparatus, which for very advanced processes is often operated at non-baseline operating conditions. The task of inventing an objective, consistent method of assigning variable ranges which are representative of a large scale facility, however, is very difficult at best for such processes. A few ideas leading toward the goal of an input determination procedure will, however, be suggested.

As a start, one can make an attempt, as in Figure 8.2, to classify the uncertain process input variables as to type and function. This task was addressed in a very general way in Chapter V. The categories discussed here are also intended to be generic for any process and also be suitable for interpretation of uncertainty analyses. The variables to be considered all fall within the three modeling classifications, $(X_i)_{perf}$, $(X_i)_{des}$, and $(X_i)_{cost}$, which were discussed in Chapter V. For this chapter, a more detailed morphology of process variables will be utilized, since the selection of the proper probability distribution depends somewhat on the variable classification.

Five general but descriptive categories of input variables are suggested: (1) process science, (2) hardware performance, (3) equipment cost, (4) operating cost, and (5) RAM variables. The first two categories affect productivity, which in turn affects unit production costs. The third and fourth do not affect productivity but affect only the total annualized cost. The last is predominantly an operating cost-related category; however, it does affect overall facility productivity via the plant availability.

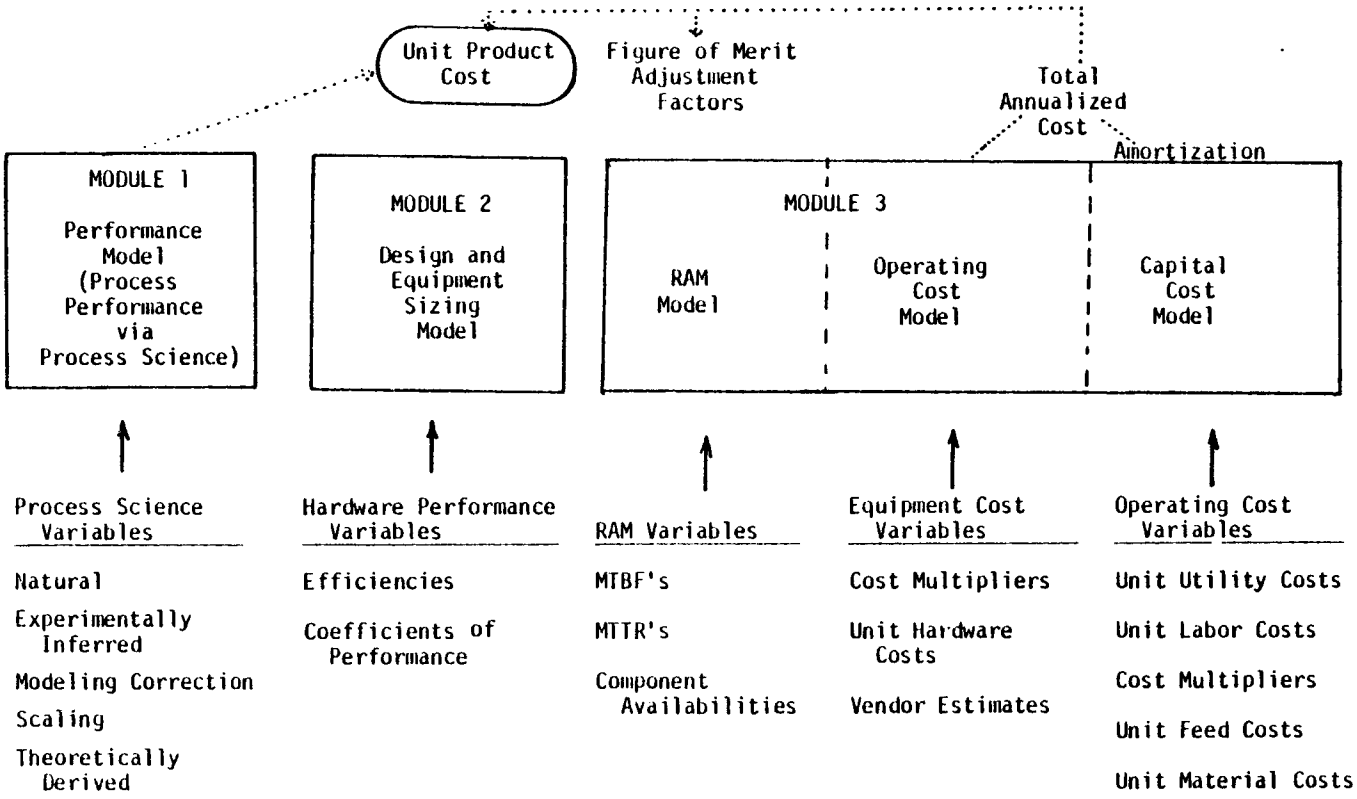


Figure 8.2

Generic Classification of Assessment Model Variables for MVSS

Each general category of variables has subcategories that are worthy of individual discussion. In some cases a variable could reasonably fall in two subcategories. In such cases one can arbitrarily assign it to one category without being overly concerned with the effects on the overall result, i.e., the result generated from running all of the input variables together.

General Category 1. Process science variables. In this category of variable, five subcategories can be identified: (a) natural parameters, (b) experimentally inferred data points, (c) modeling correction factors, (d) scaling parameters, and (e) theoretically derived parameters.

(a.) Natural variables are those for which at a given set of process conditions a single value exists in nature. Its determination, however, is subject to systematic and random error in its measurement. Many such variables depend on conditions such as pressure, temperature, magnetic or electric field strength, and particle kinetic energy, which are held constant during a given measurement. Examples of such variables would be nuclear and spectroscopic absorption cross sections, physical properties of materials, and reaction rate constants. The person making the measurement can often supply the analyst with statistical information or error bars on this type of data.

(b.) Experimentally inferred variables are those for which measurements exist from subscale or off-line experiments but which are hopefully assumed to also be correct for the baseline plant and are therefore used in the productivity model. The developer often optimistically assumes that scale-up and/or process integration will not

markedly change these numbers. Some examples of such variables are separation factors in isotope separation experiments, catalyst activities, and mass-transfer coefficients.

(c.) Modeling correction variables, discussed in the first part of Chapter VII, are multipliers used to allow for some degradation in particular productivity related phenomena for which no detailed model exists, but for which it is known that an unexplained deleterious effect is present. The use of these modeling correction variables in the productivity model is superior to trying to incorporate such uncertainties via the performance discount factor.

(d.) Scaling variables may be used in the productivity and design and equipment sizing models to account for the uncertainty in the extent of scale-up necessary to go from development size equipment to the baseline plant technology. Such a parameter could be a scaling exponent relating equipment dimensions, a multiplier accounting for material losses encountered during scale-up, or parameter correcting for duty changes imposed by changing the geometry of the particular piece of equipment. An example might be a scaling exponent utilized in calculating the stage height in the design model for a packed tower in a new separation process.

(e.) Theoretically derived variables constitute those which have not been measured (and are often extremely difficult to measure) but are derivable from theory. For example, many spectroscopic cross sections are calculable from quantum mechanical considerations. Reaction rate constants can in many cases be calculated from kinetic theory and mass-transport theory. The calculation of these values is often performed

with large, very complex computer codes which are run separately from the process productivity model.

Category 2. Hardware performance variables. Since these variables tend to be highly process-specific, this category of variables is difficult to break up into subclasses; however, one type of frequently used variable can be discussed. Hardware performance is often measured in terms of efficiencies, which in most cases are dimensionless quantities that express the ratios of some desired output quantity to an input quantity, with the difference considered a material or energy loss. The quantity considered is most often energy in some form. Efficiencies are often used to rate lasers, generators, turbines, and engines. Relationships between mass quantities and energy quantities are often expressed in terms of non-dimensionless efficiencies, such as thousands of CFM of air moved per kilowatt-hour for a fan efficiency. Values for these types of variables are frequently obtained from hardware development teams associated with a project. Optimistic boundaries for efficiency values can often be obtained by calculation of theoretical limitations. Scale-up of hardware often results in changes in efficiency which are not always for the better. Equipment sizing is heavily dependent on efficiency input information since one of the quantities that comprises the ratio defining the efficiency (most often the output or numerator) is usually fixed. For this reason process equipment power consumption requirements usually vary inversely with electrical efficiency.

Category 3. Equipment cost variables. In an advanced technology process the analyst is faced with the problem that the major process

hardware for the baseline design will represent a first use of the given technology on a large scale. For this reason there is little procurement experience on which to rely. A set of estimated costs will exist for the baseline, but these can only be considered as educated guesses by cost estimators. In order to allow inclusion of uncertainty, a multiplier on the cost of each generic type of equipment utilizing a novel technology can be used, with 1.0 constituting the baseline value. For large, single units in a facility this is a useful concept.

For multiple equipment or that designed on a "duty" or mass or energy flow basis, it is useful to consider a unit cost variable, such as dollars per kilowatt of laser light, dollars per SCFM, or dollars per watt of photovoltaic power. By assigning a range to these unit cost values, economies of scale which might be realized in the unit costs of certain items via learning effects can be handled simultaneously without requiring the use of additional learning curve algorithms. The greater the number of equipment cost uncertainties which can be handled by this subcategory of variables, the less one must rely on the capital cost growth factor, F_{CCG}.

Category 4. Operating cost variables. As with the capital costs, operating cost uncertainties are impacted by the fact that one is probably dealing with a first-of-a-kind process. Operating procedures will often represent new techniques, not tested on a production scale, and raw materials and replacement material requirements will at best be based on engineering and development estimates. The quality of raw materials cost estimates can vary from excellent (where a commodity can be bought in the marketplace) to questionable (where a new material

itself has to be developed and brought into production for this particular application).

Both raw material and replacement parts costs are best handled on a unit-cost basis. The same can be said for utility costs such as the cost of electric energy, which is expressed in dollars per kilowatt-hour. For expressing uncertainties on the cost of an operating procedure, it is useful to create a new variable which is a cost multiplier on the lumped cost of the labor and materials for the particular procedure in question. This method is less cumbersome than applying separate multipliers to each labor and material category. The more variables that can be directly handled with in the operating cost category, the less one must rely on the operating cost growth factor, F_{OCG}.

Category 5. RAM variables. Since RAM variables affect both production cost and productivity, they are considered in a separate category. The data here can consist of MTBF or lifetime estimates for the major process equipment items or components thereof which must be replaced at a frequency such that the replacement cost significantly impacts the operating costs and/or availability. If repair time or the mean-time-to-restore is calculated to have a significant impact on manpower or the number of spares required, the MTTR estimates for these equipment items should be included as an uncertainty in the analysis.

Mathematical Forms for Input Variable Probability Distributions

A primary difficulty in applying a simulation approach to new technology economic evaluation lies in developing the probabilistic input representations, i.e., distributions (or more correctly, probability

density functions or pdf's), for pertinent unit cost-driving variables. In the usual investment risk analysis applications, such as those proposed by Hertz,[76] many of the input probability distributions used in simulation studies can be developed as frequency histograms from historical or marketing data. However, since a development project is often a unique, non-state-of-the-art project, the accumulation of historical economic or productivity data is not possible. Thus, some alternative means for developing input probability distributions must be used. It should be remembered that probability distributions are in essence models from which the Monte Carlo driver code can draw samples. At the end of the simulation, each input will have its own frequency histogram which should approximate the functional form of the pdf.

In the area of investment analysis, several contributors have suggested solutions to the problem of developing probability distributions. Hertz and others[77] present the argument that probability distributions can be based on subjective judgments made by the executive decision-maker. In these procedures, three subjective estimates for each investment outcome are obtained: a most likely, an optimistic, and a pessimistic. Van Slyke[78] suggests a subjective estimation procedure similar to that used in the project evaluation and review technique (PERT) network planning process.

For a process evaluation application of this type, no robust, prepackaged procedure exists. Selection of the input numeric values defining the desired range of the distribution is the most difficult step, followed by determination of the correct type or shape of probability distribution to encompass, or in essence model, the distribution

of these values. It is the purpose of this subsection to discuss a few types of important distributions and their appropriate applications. A Glossary of Uncertainty Analysis Terms appears in Appendix C.

Distribution Parameters

The input variable probability distributions one confronts in Monte Carlo simulation represent the probability density functions (pdf's) of the random variables from which single point input values, X_i, are selected for each input ensemble, X_i submitted to the model. The pdf shows only relative probabilities. In order for the random number (a real number between 0 and 1) to be utilized, the pdf must be integrated to form a cumulative distribution function or cdf with a maximum cumulative probability of unity, i.e., the area under the pdf curve. The cdf is then algebraically inverted or transformed such that an input value or "return value" can be calculated for each cdf probability value selected between 0 and 1. This procedure is shown graphically in Figure 8.3.

During the iteration process, which really represents a sampling process from the parameter defined input density function specified, statistical data on the input sample or distribution, such as mean and standard deviation, are calculated and can be compared to the original statistical parameters which were utilized to define the pdf As the number of replications increases, the closer the sample distribution parameters are to the specified pdf parameters.

Among the parameters of interest are the mode, median, and mean of the distributions of choice. The mode represents the most frequently occurring value, i.e., the incremental range or "bin" in which the most samples fall or the maximum of the defining pdf curve. The median or

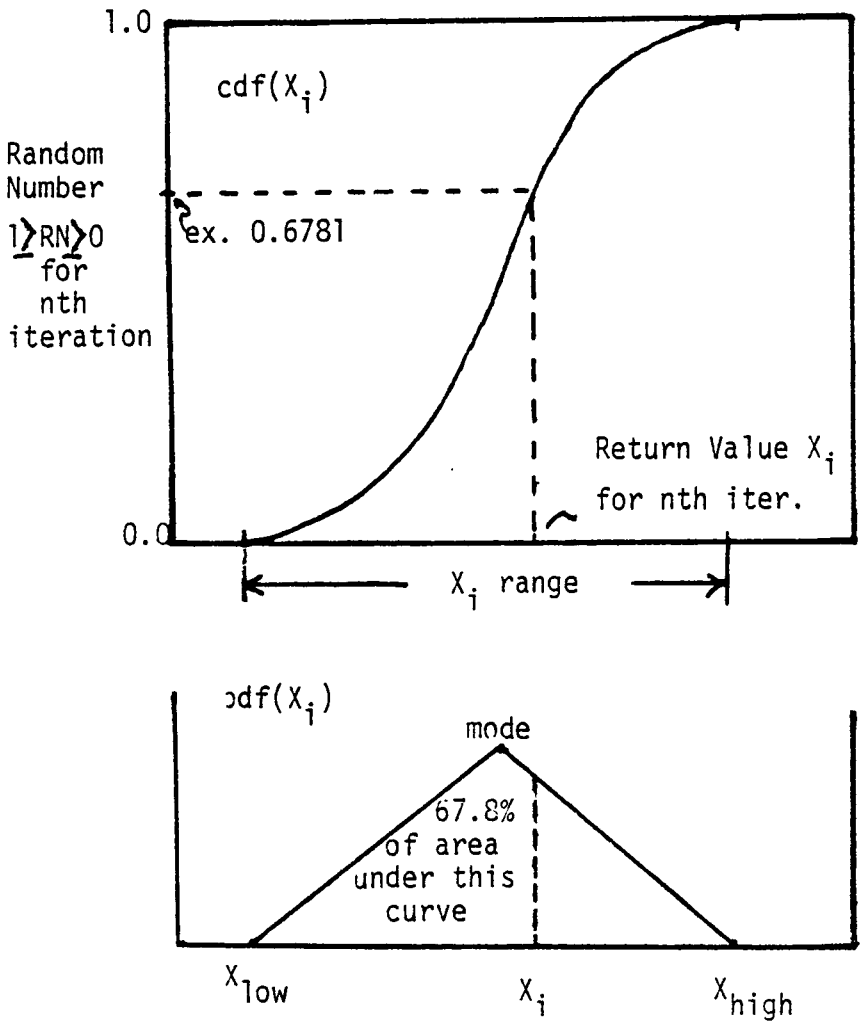


Figure 8.3

Generation of Return Values from Random Numbers and cdf's

50% percentile represents the value for which any random variable on the distribution has an equal chance of falling above or below. Half of the area under a pdf curve will lie to each side of this point. The mean represents the expected value which would be calculated from the random variables. It is calculated during the iteration procedure by taking the arithmetic mean of all the samples taken. The skewness or departure from symmetry of a distribution can be qualitatively assessed by looking at the position of the pdf mean relative to the pdf mode. The value of the mean relative to the mode is the indicator of the direction of skewness. The following definitions apply:

positive skewness: mean > mode

negative skewness: mean < mode

A dimensionless measure of skewness can be calculated as follows:

$$\text{skewness} = \frac{\text{mean - mode}}{\text{standard deviation}} .$$

The above symmetry attributes are sometimes referred to as Pearson's first and second coefficients of skewness.

Another characterization parameter is the kurtosis or "peakedness" of a distribution, expressed as the fourth moment about $\bar{x}$:

$$\text{Moment coefficient of kurtosis, } a_4 = \frac{\overline{(x-\bar{x})^4}}{\sigma^4} .$$

where σ is the standard deviation and $\overline{(x-\bar{x})}$ is the mean deviation from the distribution mean. For the normal distribution, $a_4 = 3$. A leptokurtic, or highly peaked distribution, has an a_4 value greater than 3; a platykurtic, or lightly peaked distribution, has an a_4 value less than 3.

Kurtosis is useful in comparing the shapes of distributions. The properties and uses of a few selected distributions will now be discussed, with continuous distributions to be considered first.

Normal distribution. The normal, bell-shaped, or Gaussian distribution is descriptive of the distribution obtained for most measured natural variables. The mathematical form is expressed as:

$$N(x;\mu,\sigma) = [1/(\sqrt{2\pi}\,\sigma)]e^{-(1/2)[(x-\mu)/\sigma]^2} ,$$

where:

μ = the mean of the distribution,

σ^2 = the variance (σ is the standard deviation), and

$-\infty < x < \infty$, where x is a continuous random variable.

The mean and standard deviation completely determine the distribution and are the only parameters which need be supplied in the input data. Since the domain of x extends to infinity in both directions, some truncation must be used in computer applications. The return values are limited to a range of $\pm 6\sigma$ from the mean for the Monte Carlo driver code utilized in this document. To prevent the occurrence of negative return values in this range, the lowest value a positive return value can assume is $\mu/50$. If other truncation criteria are desired, there is a special position in the input table (Appendix L) for these cases. The $\pm 6\sigma$ criterion includes 99.99+% of the points which would be represented by a normal distribution where $-\infty < x < \infty$. The return value for simulation is created by use of a function subprogram which generates normally distributed random numbers from uniformly distributed random numbers. The subprogram utilizes the principles of the Central Limit Theorem by

summing enough uniformly distributed random numbers (12 in this case) to approximate a normal distribution. The use of the normal distribution, by definition, implies that some type of measurement, sample, or historical data are available to the analyst. Even though only two parameters are needed to define it, the user also assumes that the information one plans to input inherently fits this type of curve.

Log-normal distributions. The parameters for the log-normal distributions are similar to the normal distribution. If one considers a random variable x where $Y = \ell n\ x$ is normally distributed with mean μ_Y and variance σ_Y^2, a logarithmic transformation to obtain μ_X and σ_X^2 in terms of x is necessary:

$$N(x;\mu_X,\sigma_X) = [\frac{1}{x\sigma_Y\sqrt{2\pi}}]e^{-(1/2)[(\ell nx-\mu_Y)/\sigma_Y]^2} .$$

The parameters of this distribution and other commonly used distributions are summarized in Table 8.1. This distribution is positively skewed and is often used in econometrics and for the representation of time distributions in queueing problems. For application in process uncertainty analysis it can be useful for representing natural parameters whose measured values span more than one order of magnitude, such as spectroscopic cross sections.

Triangular distribution. The triangular distribution has the advantage that any degree of skewness can be easily represented. This is the situation represented when the mode differs from the median or mean. Triangular distributions are defined by a minimum, mode, and maximum value. The minimum and maximum are absolute, i.e., they do not

Table 8.1

Parameters of Commonly Used Continuous and Discrete Probability Density Functions

Name	Symbol	Domain	Restriction	Mean	Variance	Mode
Continuous Distributions						
Beta	$\beta(a,b)$	$0\le x\le 1$	$a,b>0$	$\frac{a}{a+b}$	$\frac{ab}{(a+b+1)(a+b)^2}$	$\frac{a-1}{a+b}, a\ge 1$
Exponential	$E(\beta)$	$0\le x\le\infty$	$\beta>0$	β	β^2	0
Gamma	$G(\alpha,\beta)$	$0\le x\le\infty$	$\alpha,\beta>0$	$\alpha\beta$	$\alpha\beta^2$	$(x-1)\beta, \alpha>1$
Lognormal	$LN(\mu,\sigma^2)$	$0\le x\le\infty$	$\sigma^2>0$	μ	σ^2	$e^{\mu-\sigma^2}$
Normal	$N(\mu,\sigma^2)$	$-\infty\le x\le\infty$	$\sigma^2>0$	μ	σ^2	μ
Triangular	$\Delta(a,b,c)$	$a\le x\le c$	$c>b>a$	$\frac{a+b+c}{3}$	$\frac{a(a-b)+c(c-a)+b(b-c)}{18}$	b
Uniform	$U(a,b)$	$a\le x\le b$	$b>a$	$\frac{a+b}{2}$	$\frac{b-a}{12}$	(a,b)
Weibull	$W(\alpha,\beta)$	$0\le x\le\infty$	$\alpha,\beta>0$	$\beta\Gamma\left(\frac{1}{\alpha}+1\right)$	$\beta^2\left[\Gamma\left(\frac{1}{\alpha}+2\right)-\Gamma^2\left(\frac{1}{\alpha}+1\right)\right]$	$\left(\frac{\alpha-1}{\alpha}\right)^2\beta, \alpha>1$
Discrete Distributions						
Binomial	$Bi(n,p)$	$0<p<1; n=1,2,\ldots$	$x=0,1,\ldots,n$	np	$np(1-p)$	-
Geometric	$Ge(p)$	$0<p<1$	$x=0,.,\ldots,\infty$	$\frac{p}{1-p}$	$\frac{p}{(1-p)^2}$	-
Hypergeometric	$Gh(n_1,n_2,x)$	$x=1,\ldots,n_1+n_2$	n_1,n_2 integer	$\frac{xn_1}{n_1+n_2}$	$\frac{xn_1n_2}{(n_1+n_2)^2}\left(\frac{n_1+n_2-x}{n_1+n_2-1}\right)$	-
Poisson	$P(\beta)$	$\beta>0$	$x=0,.,\ldots,\infty$	β	β	
Uniform	$U_d(a,b)$	$b>a$	$x=a,\ldots,b$ a and b integer	$\frac{b+a}{2}$	$\frac{(b-a)(b-a+2)}{12}$	-

have the long, low probability tails which characterize the normal and exponential distributions.

Figure 8.4 illustrates that an isosceles (symmetric) triangular distribution is an approximation to the middle portion of a normal distribution, i.e., a normal distribution without the long tails. The endpoints (minimum and maximum) represent ±2.1 standard deviations or sigmas (2.1 σ's) from the mean of a normal distribution, which would include 96% of the area under the normal curve.

MacCrimmon and Ryavec[79] in a comparative analysis of several distributions, discuss the popularity of the triangular distribution with decision makers and analysts. Because of the ease with which the triangular distribution can be comprehended by decision makers and implemented by the analyst, it is used frequently in the examples presented in this study.

Three subjective estimates of each input variable are used to form the triangular distributions. Generally speaking, the optimistic estimate is the range endpoint value which would produce the lowest unit cost if a single variable sensitivity analysis were performed over the entire range of the distribution. This is the result which might be experienced if good luck is experienced and everything in the development program goes right. The pessimistic estimate represents the opposite outcome, a result which can occur if development disappointments are experienced. The pessimistic value should reflect the possibility of numerous technological and implementation problems occurring in the development project; however, it should still represent valid input to the baseline technology model it drives. The most likely or modal estimate is the "best guess" value for the parameter of interest. This

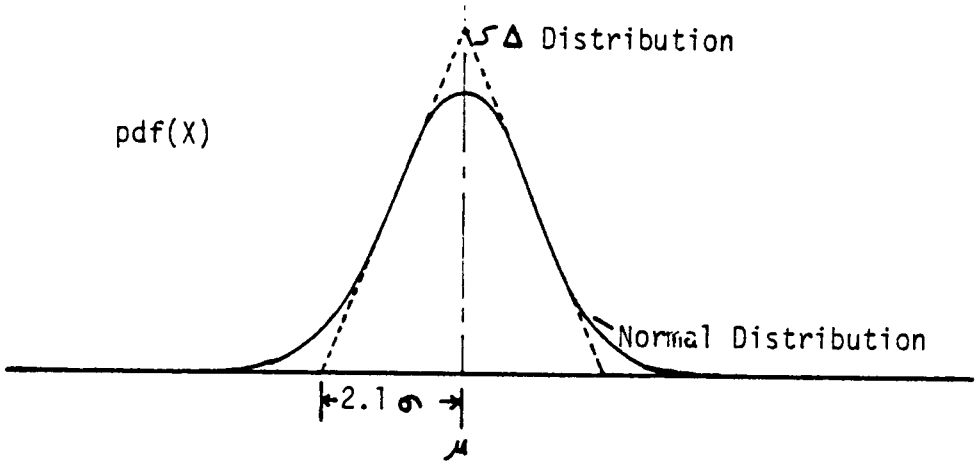


Figure 8.4

Comparison of the Normal and Triangular pdf's

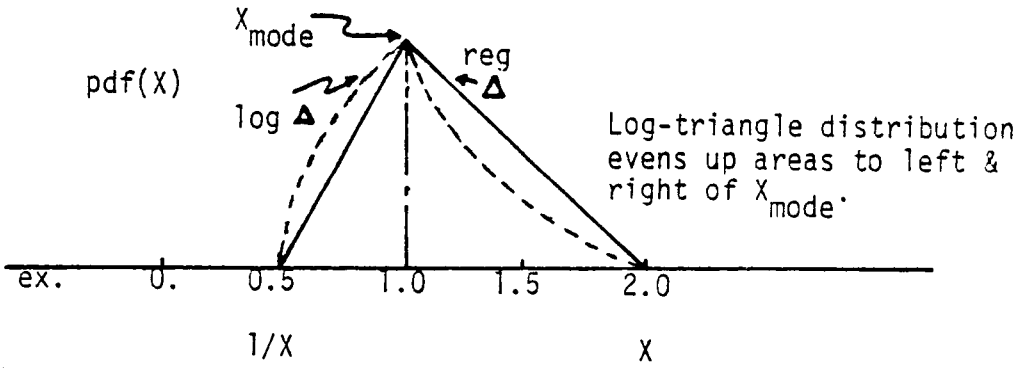


Figure 8.5

Properties of the Log-Triangle pdf

estimate should be expected to appear most frequently over the population of all ensembles during the course of the simulation. This value can be, but is not necessarily, the baseline input value $(X_i)_{base}$. The statistical parameters such as μ and σ for the triangular distribution are also listed in Table 8.1 but are not needed to define it. This fact by itself adds to its appeal to decision makers. Control of skewness can gauge the evaluator's degree of optimism or pessimism concerning the range of a given variable; for example, experience indicates that hardware cost variables are more likely to increase than decrease, hence an input unit cost distribution is generally skewed toward values above the input mode. The "skewness" of the input curves has a strong effect on the location of the median of the output histogram distribution relative to the output mode for the process figure of merit.

Log-triangle distribution. The relationship between the log-triangle and triangle distribution is analogous to that between the normal and log-normal distribution. By use of a log-triangle distribution, which appears as a triangle with a slightly curved side as in Figure 8.5, one can arbitrarily pick a mode and two endpoints and force the mode and median to be fairly close together, especially when input data span orders of magnitude. This latter type of distribution is frequently employed for theoretical process science variables used in productivity models. This distribution is also useful for variables used as multipliers which lie on both sides of a mode of 1.0. It has the property that the mode and median are the same if distribution range endpoints 1/X and +X are used (X is a multiplier times a fixed value.)

Other distributions based on three parameters. Several alternative probability distributions can be defined by three subjective parameters (not the same as those for the triangular distribution) and fitted to the following distributions. For stoichastic PERT analysis[80] a Beta distribution is defined by three parameters to represent the time duration for the completion of a given activity in a network. Another such distribution, utilized in benefit-risk analysis and reliability studies, is the Weibull distribution. The disciplines of reliability analysis and queueing theory make frequent use of dynamic Monte Carlo simulation and require the use of computer-generated variables from many different distributions.

Fishman[81] discusses in detail the mathematics required to produce exponential, gamma, beta, Weibull, and many other continuous and discrete distributions used in reliability studies for failure simulation.

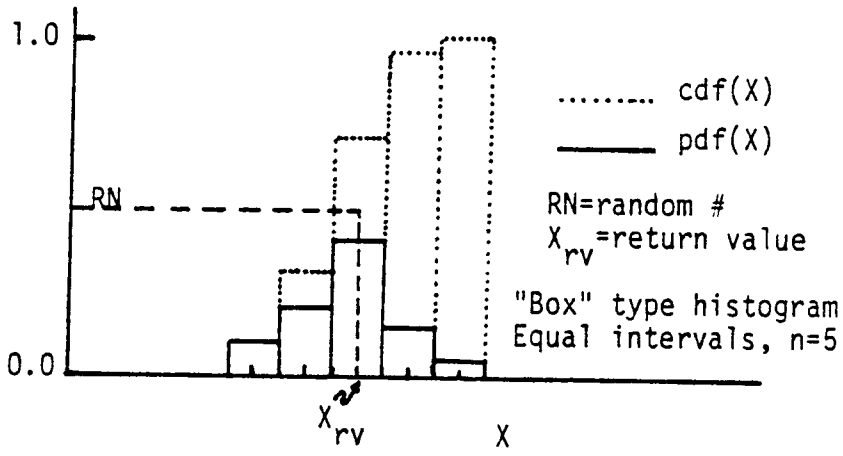
Other continuous distributions. The following distributions, like the triangular, are mentioned because of their mathematical simplicity and intuitive appeal to the analyst.

The uniform distribution. If a variable has an equal probability of occurring over the range of interest, its distribution can be represented as a horizontal line or flat distribution. This type of distribution is used where a most probable value is not known but for which the variable range can be determined.

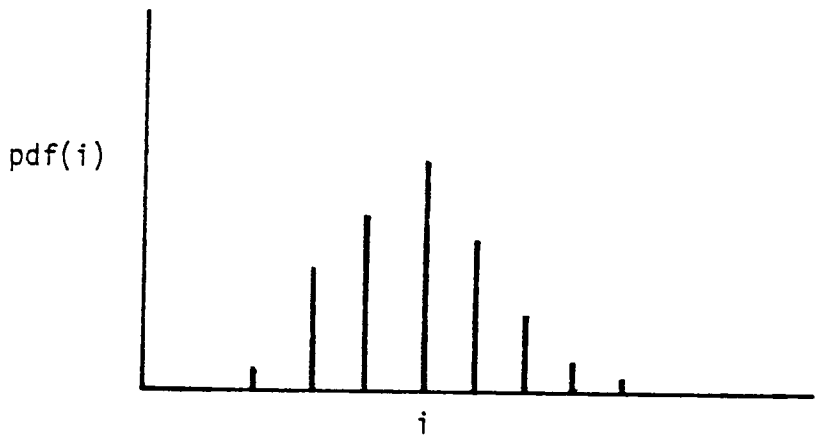
Trapezoidal distribution. The trapezoidal distribution requires four values for its determination and is a hybrid of the triangular and uniform distribution.

Discrete distributions. If one cannot find a continuous pdf which represents his data, the use of a spike-histogram or a discrete distribution is warranted. Discrete distributions are also often used where integer quantities are considered. Some of the more mathematically complex ones require that the analyst have some intuitive reason to apply and fit the distribution to a particular class of data. Among such distributions are the binomial, geometric, hypergeometric, and Poisson distributions. Others, such as the histogram distributions described below, can be used in a more subjective manner and can be easily constructed by the user of this methodology. Table 8.1 also lists the statistical parameters for a number of discrete distributions.

Histogram distributions. Two types of histogram distributions are considered. In the "box" type histogram shown at the left of Figure 8.6 only discrete values or ranges of the random variable exist, i.e., n equals the number of boxes. If the intervals of each box are equal, the cumulative distribution is easily calculated by summation and the return value X_{rv} is found by checking to see which cumulative histogram box the random number will intersect and then supplying the midpoint of that range on the integer X_{rv} as a return value. When adjacent box-type histograms are used, one is really dealing with several adjacent uniform distributions. A truly discrete histogram is represented by a plot consisting of probability "spikes," also shown in Figure 8.6 and discussed in the previous paragraph.



"Box" type Histogram Showing
pdf and cdf.



Discrete Histogram pdf for
Integer Variables

Figure 8.6

Histogram pdf's

Selection of Numerical Input MVSS Values

Since the results obtained from any simulation are only as good as the input data, the quantitative determination of MVSS input variables is of paramount importance to a process evaluation. Unfortunately, there is no clear-cut or robust procedure which guarantees consistency and accuracy in the selection of input parameter values. This is an especially serious problem where comparison of competing processes is in progress, and where consistency of evaluation must be maintained in order to protect the evaluator's objectivity and fairness.

Since many inputs require projection of what their values will be at the time of large-scale process implementation, the evaluator finds himself in the realm of technological forecasting and can benefit from exploring what this relatively new heuristic science can offer as an aid to input selection. The most useful general principle gleaned from the literature is that of collective judgment utilizing expert opinion. Policymakers often use formalized procedures, such as Delphi, to obtain a qualitative view of future development trends. Anonymity is maintained among participants, and written viewpoints are exchanged until a statistically significant consensus evolves. In this manner no well-known or dominant individual can persuade others on the basis of his standing in his field alone.

For the quantitative task at hand of determining MVSS input variables, consistency of evaluation and assignation is more important than consensus and the associated participant anonymity. Since ranges rather than single values are to be determined, consensus need not focus on one value, but rather whether the range of input values is indeed

possible. Less formal face-to-face discussion and debate among peers with a consistent set of ground rules has been found to be a useful procedure and was successfully used as part of the selection procedure for the Department of Energy's choice of an advanced isotope separation process for uranium enrichment. The "peers" in this case consisted of technical personnel from DOE and the participating development and process evaluation contractor organizations: Los Alamos National Laboratory, Lawrence Livermore National Laboratory, TRW Corporation, and Union Carbide Corporation-Nuclear Division.

The primary task of a peer review is to sort out the important technology and production cost issues from the insignificant issues which might be erected by competitors as diversions to delay considerations of technical areas where real problems exist in their own processes. Participants in such a venture must have access to technical documentation and relevant experimental data for the alternative processes. If alternative processes are not being considered, peer review among the various project teams working on a single process can still be useful as a preliminary to uncertainty analysis. Such a procedure can be instituted among R&D, engineering design, cost estimating, and operations analysis teams. Each group represents expertise in different process areas, and opinion may vary widely.

Once the peer review has identified the important issues, the analyst must submit the values going into the process model and the model itself to peer review. Although the latter task may be time-consuming, it is important that all participants have confidence that the models adequately represent the processes and cause/effect relationships

considered. Since first-of-a-kind processes vary so widely in their descriptions and relevant phenomena, no generalized quantitative rules can be set forth for assigning input ranges. Along with the qualitative properties of the various previously discussed probability distributions, the following guidelines are given for assignment of numerical values:

1. Input ranges should be maintained within the realm of the baseline technology. As an example, a temperature too high for use in the baseline technology should not be included in the temperature range.

2. Inputs should remain within the reoptimization capabilities of the model. Failure to do so will result in physically unreasonable results or possible program execution problems in the optimizer part of the overall set of modeling algorithms.

3. The mode input values do not have to correspond to the base or reference case. The analyst must determine the reasonableness of the baseline inputs and keep in mind that a baseline supplied by a development organization is likely to include optimistic values; however, there are cases in which a confident developer might submit an overly conservative baseline. In a report by Iversly and Kakneman,[82] the tendency of estimators, regardless of their sophistication, to state overly narrow confidence intervals is discussed. Iversly and Kakneman believe this tendency is due to a heuristic of thinking common to all people that an estimator anchors the expected range to the original best estimate chosen by the estimator.

4. Even if all the input distributions have as their mean the baseline value for each input, the Monte Carlo driver or sampling

program will never reproduce the base case exactly, i.e., no single design is produced in which all the input distributions have their baseline values chosen by the random number generator.

5. It should be verified that hardware component costs reflect an uncertainty consistent with their state of development.

6. It should be qualitatively ascertained whether any ensemble of random input variables selected by the Monte Carlo driver might represent an inconsistent or physically non-realizable set of input data. If so, there are dependencies between variables or logic problems within the code itself which need correction. By printing out the input distribution return values and output figures of merit every couple of iterations, one can get ensembles of data to inspect for possible problems of this nature. L. Kryzanowski et al.[83] suggest a means of handling dependencies between variables which impose conditional probabilities via "base" and "keyed" variables.

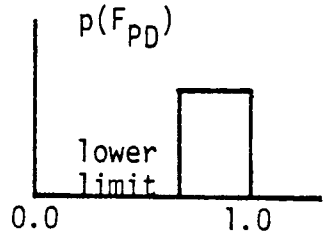
7. For less vowel hardware items a capital cost uncertainty criteria based on procurement history, if available, similar to that used for estimating contingency might be used for the assignment of cost ranges.

Distributions for Figure-of-Merit Adjustment Factors

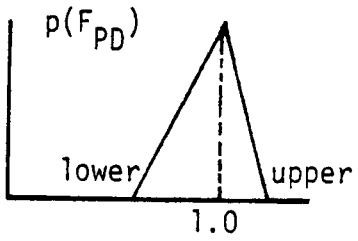
The four global adjustment factors--performance discount, capital cost growth, operating cost growth, and project delay penalty--may also be input variables to the total MVSS and can have distributions associated with them. The determination of upper and lower values for their ranges was briefly discussed in Chapter VII. As with the determination of their limits, the determination of the shape of the

distribution will require considerable subjective judgment. The net result of utilizing distributions on the factors in a simulation is a shifting and reshaping of the unit cost output distribution obtained when the process is simulated without adjustment factors. For this reason the input shapes of the adjustment factor distributions will strongly influence the parameters of output the distribution for the unit cost. The input distributions are discussed below. It should again be mentioned that the use of these factors and their distributions is allowable only for the earliest models.

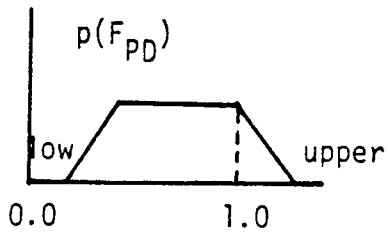
Distribution of the performance discount factor. Having determined the upper and lower limits on the performance discount factor, one must now give some indication of the likelihood that these values and those between these limits and the baseline will be realized. Figure 8.7 shows a few sample distributions. If one believes that the lower limit and all other values up to 1.0 have an equal probability of occurring, then a uniform distribution would be suitable. The triangular distribution is useful where the upper and lower limits have a small probability of occurrence. A trapezoid can be used where attributes of both the triangular and uniform distributions are desired. Since determination of F_{PD} is very subjective, it is inappropriate to use mathematically complicated distributions such as the normal which fit only particular types of data. If there are no backup technologies or alternatives which might increase performance over that predicted by the model, an F_{PD} value of 1.0 will constitute the upper limit and likely mode of this distribution. A lower mode value would indicate that performance degradation is more likely to affect the baseline than not. The skewness of



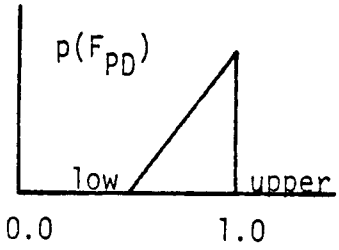
(Uniform dist.,equal probabilities)



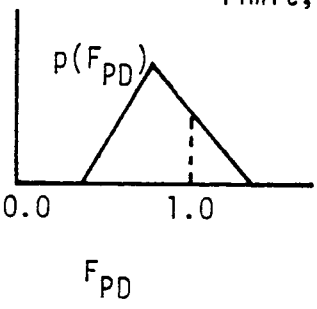
(Triangle dist, ref.case is most likely)



(Trapezoidal dist.)



(Reference perf. is upper limit, no process backups)



(Mode F_{PD} 1, perf. degradation more likely than not)

Figure 8.7

Example Distributions for the Performance Discount Factor

this distribution about the baseline (FPD = 1.0) will determine the extent to which the F_{PD} adjusted simulation output mean will shift relative to the output mean obtained in a simulation with no F_{PD} distribution applied.

Distribution of the cost growth and project delay penalty factors. These distributions are included in a single discussion since their properties are similar. The problem addressed here is to express the likelihood of cost growth or project construction delay occurring relative to the likelihood of the costs and the interest during construction coming in at values predicted by the economics model alone. If the analyst determines that cost growth (and/or IDC growth due to project delay) is just as likely to occur as not, a uniform distribution spanning the range from the base case ($F_{CCG} = F_{OCG} = F_{PDF} = 1.0$) to the upper limit for each factor is warranted. Trapezoidal or triangular distributions can be used for cases where unequal likelihoods are to be expressed as was done for F_{PD} in Figure 8.7.

In most cases these distributions will be positively skewed, i.e., cost growth or project delay is more likely to occur than cost underruns or early project completion. The net effect will be to shift the output mean unit costs upward from the case where $F_{OCG} = F_{CCG} = F_{PDF} = 1.0$.

Application of the Monte Carlo Technique

Advantages of Multivariable Sensitivity Study (MVSS) Methods

Most preliminary assessments for new processes do not consider the problem of establishing uncertainties for the desired economic figures of merit but rather focus only on a single baseline representation

of the process. For most new processes an attempt is usually made in early assessments to identify those variables which exhibit significant leverage on the figures of merit by means of varying process input variables one at a time (SVSS). Such sensitivity studies may be used to define the range of expected outcomes but they do not provide a measure of the likelihood of any particular outcome or range of outcomes. Analytical and statistical methods for MVSS provide an alternative to the single-point baseline characterization which can be used to calibrate the relative optimism of baseline assumptions within the available physics/chemistry/engineering/economic milieu.

Before discussing implementation of the Monte Carlo method it is of interest to consider analytical methods for handling probabalistic uncertainty data in models. From this, one can gain an understanding and appreciation for the power of the Monte Carlo method in making uncertainty assessments for immature processes.

An Analytical Method

Since the Monte Carlo simulation method is an iterative computation method and can involve considerable machine computation time, an analytic method should be used whenever possible. Unfortunately, few models have the simple algorithmic forms desirable for application of the propagation of variance method described below. The algebra of the statistical moments (mean, x, and variance, σ^2) of normal distributions is well documented in statistics texts. The mean or expected value of an output function is simple to calculate since it merely represents the same functional relationship applied to the input means as was applied to the random variables from each input variable pdf. Variances,

however, have a more complex algebra depending on the arithmetic operation within the function, and this complexity represents the main limitation of analytical methods. The following example shows the relationship for $f = f(x_1, x_2, \ldots x_i)$ and the associated variances, σ_i^2, and means x_i:

For $f = x_1 + x_2 + x_3 + \ldots x_i$,

$$\sigma^2(f) = \sigma_{x_1}^2 + \sigma_{x_2}^2 + \sigma_{x_3}^2 + \ldots \sigma_i^2 \quad \text{(additive property).}$$

For $f = x_1 x_2$ (i limited to 1 and 2 for sake of simplicity),

$$\sigma^2(f) = \bar{x}_1^2 \sigma_{x_2}^2 + \bar{x}_2^2 \sigma_{x_1}^2 + \sigma_{x_1}^2 \sigma_{x_2}^2 .$$

For $f = x_1/x_2$, i limited to 1 and 2,

$$\sigma^2(f) = (\bar{x}_1^2 \sigma_{x_2}^2 + \bar{x}_2^2 \sigma_{x_2}^2)/\bar{x}_2^4 .$$

Another limitation on this method, as with other uncertainty analysis methods is the requirement that the input variables x_i be statistically independent, i.e., that no functional relationships or correlations exist between any of the inputs. If the inputs are not independent, covariance terms must be added to the expression. For the simplest case of a sum $f = x_1 + x_2$,

$$\sigma^2(f) = \sigma_{x_1}^2 + \sigma_{x_2}^2 + 2\ \mathrm{cov}(x_1 x_2) .$$

Calculation of the covariance term requires a knowledge of the relationship between the inputs. The correlation coefficient r is often used for this purpose where

$$\mathrm{cov}(x_1 x_2) = r\ x_1^2\ x_2^2 .$$

The problem of statistical bias in modeling introduced by variable dependency is discussed by Kryzanowski et al.[84] and Hull.[85]

The worst limitations of this analytical method are that in most models there is significant complexity, and the mathematical expression needed to evaluate a complicated function of several variables makes calculations very cumbersome. Analytical methods are most often used in additive type models, such as the calculation of cumulative measurement errors. The fact that symmetric normal pdf's must be used is another shortfall. For many inputs a skewed pdf or a non-analytic histogram pdf is more appropriate. The Monte Carlo method overcomes all these problems except that of dependent input bias. Careful choice of input variables, careful model construction, and compensation techniques suggested in the literature[86][87] can minimize these effects.

A Statistical Method: The Monte Carlo Technique

Monte Carlo simulation methods can provide probability distributions for process figures of merit by making repeated evaluations of the system response using input variable values drawn randomly from appropriate pdf's that represent the statistical properties of each input variable. After performing a large number of such evaluations a statistical distribution or histogram of system response is obtained. Meaningful use of the Monte Carlo method only requires a systems model adapted to the required inputs and pdf's of the inputs which represent both possible and probable outcomes.

The Monte Carlo simulation procedure consists essentially of five steps. Figure 8.8 shows a flowchart for the simulation procedure.

1. Input: For each input variable, X_i, a distribution must be defined which gives the probability of occurrence for any particular

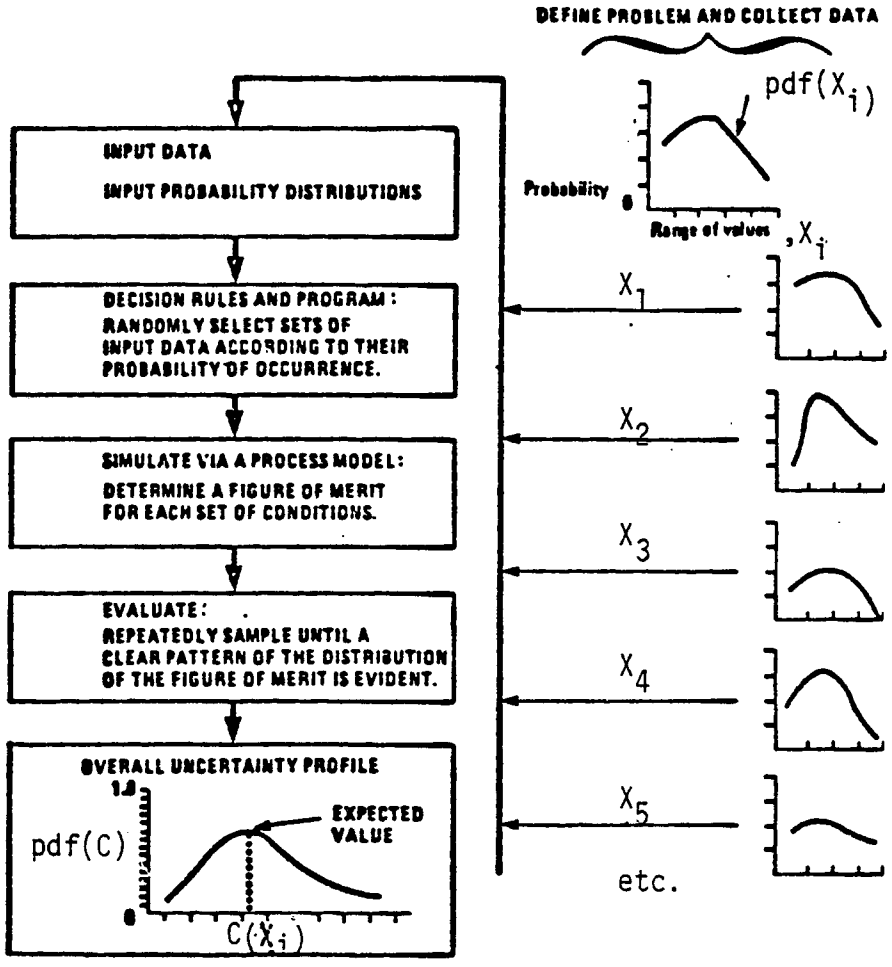


Figure 8.8

Flowchart for Simulation Procedures to Evaluate a Process Subject to Multiple Uncertainties

value within the variable range. It should be noted that most Monte Carlo users utilize the term "distribution" to refer to a probability density function (pdf). The types of distributions for each variable need not be the same. The subject of determining the distribution type and input values for a given variable was discussed in an earlier subsection.

2. Sampling: Via a random number generator and the input distributions the computer generates an ensemble, X, of randomly selected values for each input variable chosen. Each ensemble of values is unique and represents a different possible set of occurrences. A different set of randomly chosen input values is generated for each iteration or execution of the overall code. The baseline or reference case will never be exactly reproduced in this process.

3. Simulation: The model now calculates single values of the figures of merit and other design variables internal to the model whose ultimate distributions are desired by the analyst. It is assumed that the ensemble of input variables is internally consistent and does not represent a physically impossible or unreasonable situation, especially in the case of process performance models. If so, the model should be corrected to discard or properly reoptimize such cases.

4. Iteration and Storage: Once a figure of merit is evaluated, it is stored and another ensemble of values is input to the model. The number of iterations or cases needed is somewhat model dependent. If an input ensemble consisting of the means for each input distribution is evaluated by the model (a separate calculation from the simulation) a mean output value results. If during the simulation the output values

for each figure of merit are stored and the statistical mean for all iterations is recalculated after each additional iteration, it will be found that this mean will eventually approximate the calculated mean evaluated off-line using the input distribution means. For models in which significant internal reoptimization takes place during every iteration, the difference between the statistical mean of the outcome and the mean calculated from the input means will tend to be larger than in models in which no reoptimization is present. Iteration can be cut off when the difference between the two output means reaches an arbitrarily small fraction of the off-line calculated mean. Experience indicates that for most complex models at least 500 evaluations or iterations are needed. Using additional evaluations improves the statistics and the geometrical appearance (shapes) of the input and output distributions; however, the price in machine computation time and computer input-output time can be high.

The Monte Carlo Driver Code

The Monte Carlo part of the overall code is referred to as the "driver" code since it is merely a means of submitting input and displaying output and is not process specific. This code used was written by L. M. Rosenbaum at the Union Carbide Corporation Nuclear Division. The important attributes of the code are as follows:

1. The number of input distributions plus the number of output distributions must be 100 or less.

2. Up to 999,999 iterations are allowed.

3. The code presently has six types of input distributions built in (not including the option to use a single value or constant distribution). These are triangle, normal, truncated-normal, log-triangle, trapezoid, and box-type histogram distributions.

4. Variable names must use FORTRAN naming conventions and be of size REAL*4.

5. The process assessment model (performance, design, and cost scaling) are subroutines called by the Monte Carlo MAIN program via a control SUBROUTINE named FUNCT.

Appendix L shows the input instructions and simple data set examples for the Monte Carlo driver code. Appendix M contains a FORTRAN listing of the Monte Carlo driver code.

CHAPTER IX

INTERPRETATION AND ANALYSIS OF SIMULATION OUTPUT DATA

Analysis of Modeling Outcomes

The Monte Carlo simulation technique allows consideration of hundreds of different off-baseline cases. If the analyst wishes, he could examine every case individually by printing out full output tables every iteration or case that represents submission of a new set or ensemble of X_i values. In reality he is probably interested only in output of a limited number of crucial variables. Fortunately the user has the option of choosing whatever variables he desires for display and analysis. The array of specified output values, $Y_{i,m}$ ($i = 1$ to N, $m = 1$, M; where N = total number of variables, M = number of iterations) are stored for each iteration of the simulation. At the end of the simulation (M iterations), a very large array Y of dimensions $M \times N$ is available for statistical analysis and plotting of histograms. The Y_i values stored can be input X_i, internal Q_i, or figure-of-merit variables.

Input Variables

By saving the actual X_i values sampled by the random number generation, the user can check how well the total input samples drawn approximated the input probability density function chosen. If the approximation is poor, i.e., the statistical parameters for the sample and input distribution definition differ significantly, then the user must

specify more iterations or correct the function that generates the return values from each random number.

Intermediate Variables

There is a category of internally calculated model results which one might classify as intermediate variables, Q_i, which might be of interest to the analyst as an aid to understanding the behavior of the more global figures of merit. These intermediate variables, such as yields, equipment sizes, flow rates, and specific categorical costs, are important productivity driving and cost driving variables which are generated internally by the model from the input variables. Along with the figures of merit a given intermediate variable can have its own set of statistics generated by the simulation. Although not necessarily figures of merit in the broad sense, instructions for their display as simulation outputs can be submitted with the Monte Carlo input data set (Appendix L).

Figures of Merit

These variables describe the performance and aggregated costs of the process. For the examples considered in this document, the unit cost of product is the principal figure of merit. It is useful to also display the capital cost and average operating cost histograms for the process plant.

The Generation of Output Histograms

The set of Y values generated by the simulation essentially represents the collection of M (number of iterations) responses per Y_i value obtained by the submission of M sets of deviations or sets of non-baseline inputs, X_i, submitted to the overall model.

This output data is best understood if plotted in the form of a probability distribution or pdf. These distributions take the form of N histograms constructed from the Y array. If small equal size bins of width $\Delta Y_{i,m}$ are specified for a given Y_i, each $Y_{i,m}$ value out the total of M can be assigned to the bin which contains the boundaries that encompass its value. The result is a histogram as shown in Figure 9.1. (This histogram is one particular MVSS discussed in Appendix I.) If the particular Y_i is a function of two or more input variables, i.e., $Y_i = Y_i(X_1,X_2)$, the output histogram will take the shape of a skewed bell-shaped or symmetric normal distribution. This fact is true regardless of the geometric forms of the input distributions (X_i) submitted to the model and is a consequence of the Central Limit Theorem of statistics.

An advantage of computer modeling is that in addition to performing the performance, design, and cost-scaling tasks, the computer can also perform the plotting and output data analysis task. The computer calculates the statistical parameters such as standard deviation, median, mean, and selected percentile probability ranges all specified variables, Y_i.

The 5 and 95 percentiles for each histogram are most useful since the analyst is most often interested in the middle 90% range of an output distribution. For a normal distribution these percentiles approximate the $\pm 2\sigma$ region. For this type of analysis, there is little danger in disregarding the cases representing the 5% "tails" at each end of the output histogram. These points represent highly unlikely cases or

500 POINT HISTOGRAM * = 2 POINTS

PROB	CUME	VALUE		
0.0300	0.0000	190.0	15	********
0.2000	0.0300	200.0	100	**
0.1860	0.2300	210.0	93	**
0.1200	0.4160	220.0	60	******************************
0.1140	0.5360	230.0	57	*****************************
0.0680	0.6500	240.0	34	*****************
0.0560	0.7180	250.0	28	**************
0.0360	0.7740	260.0	18	*********
0.0380	0.8100	270.0	19	**********
0.0220	0.8480	280.0	11	******
0.0220	0.8700	290.0	11	******
0.0120	0.8920	300.0	6	***
0.0140	0.9040	310.0	7	****
0.0160	0.9180	320.0	8	****
0.0100	0.9340	330.0	5	***
0.0120	0.9440	340.0	6	***
0.0120	0.9560	350.0	6	***
0.0020	0.9680	360.0	1	*
0.0020	0.9700	370.0	1	*
0.0000	0.9720	380.0	0	
0.0020	0.9720	390.0	1	*
0.0040	0.9740	400.0	2	*
0.0040	0.9780	410.0	2	*
0.0000	0.9820	420.0	0	
0.0020	0.9820	430.0	1	*
0.0020	0.9840	440.0	1	*
0.0000	0.9860	450.0	0	
0.0000	0.9860	460.0	0	
0.0020	0.9860	470.0	1	*
0.0040	0.9880	480.0	2	*
0.0040	0.9920	490.0	2	*
0.0000	0.9960	500.0	0	
0.0000	0.9960	510.0	0	
0.0000	0.9960	520.0	0	
0.0000	0.9960	530.0	0	
0.0000	0.9960	540.0	0	
0.0000	0.9960	550.0	0	
0.0000	0.9960	560.0	0	
0.0020	0.9960	570.0	1	*
	0.9980	580.0		

Photochemical S Removal
MVSS #2 : F_{PD} & F_{CCG} included

STATISTICS FOR OUTPUT VARIABLE TON (Unit Cost of Methanol, $/ton)

MINIMUM 191.40 MAXIMUM 612.30

MEAN 243.89 VARIANCE 2864.0 STD.DEVIATION 53.516

PERCENTILES: 2.5% 198. 5.0% 201. 50.0% 227. 95.0% 345. 97.5% 400.

Figure 9.1

Output Histogram Resulting from Use of Monte Carlo Procedure

combinations of input variables. By dealing with the middle 90%, the user is considering the most representative cases or outcomes.

It should be noted that the most probable, i.e., $(X_i)_{mode}$, values used for the input distributions are not necessarily the inputs $(X_i)_{base}$, defining the baseline case. Even if $(X_i)_{base}$ and $(X_i)_{mode}$ are equivalent, the single-point baseline case itself is never reproduced during simulation, although several cases which have output figures of merit close to the base case figure of merit are likely to be generated.

In many cases discontinuities, raggedness, or "spikes" will occur in the output histograms. Two causes contribute to this appearance--poor input statistics and/or the existence of discontinuous functions within the model itself. If a large number of evaluations are used, the former factor will have a reduced effect; however, the latter can arise as a result of reoptimization in the model and the fact that many entities in the model must occur as discrete or integer quantities (e.g., number of process units). As an example, capital costs often huddle around values proportional to the number of process buildings or units. Design/economic relationships are seldom smooth over the entire region of interest.

Interpretation of the output statistics and histograms will now be discussed.

Location of the Best-Guess Figure-of-Merit Estimate Relative to Probabilistic Figure-of-Merit Data

For processes in the early RD&D stages economic risk may be defined as the likelihood that the process will not reach the economic goal

established by the process proponent, i.e., the predicted unit production cost. Note that this definition of risk is not exactly the same as that for uncertainty, although the words are frequently synonomous in common usage. The proponent's single-point, model generated figures of merit for the baseline design, along with associated best-guess single-point input values which support it, are sometimes referred to as the "base case," "baseline," or "point design."

If ensembles of data ($X_{i,m}$) from sampled input distributions (rather than one set of single-point values) are fed to the process model, the array representing the figures of merit (e.g., unit costs) calculated is displayed in the form of a probability histogram which approximates the shape of a normal distribution. The baseline figure of merit can be respresented as a spike or single point value on the same abscissa as the histogram. Figure 9.2 illustrates such an example. Since the area under a probability density function has a value of 1.0, the fraction of the area that lies above the base case value can be said to be a representation of the risk that a process will not meet its unit cost goals. Conversely, the probability of success may be defined as the area lying to the left (i.e., lower unit cost) of the base case. This left-lying area can be used along with other strategic planning data, if available, such as pricing and demand information, to give a measure of the process benefit to the enterprise. Such an analysis would constitute a separate evaluation task.

If one defines future project success as the attainment of a given baseline unit cost, $C_{U,\,base}$ (most often representing inputs submitted to the model by a process proponent), one can integrate the curve pdf(C_U) from its

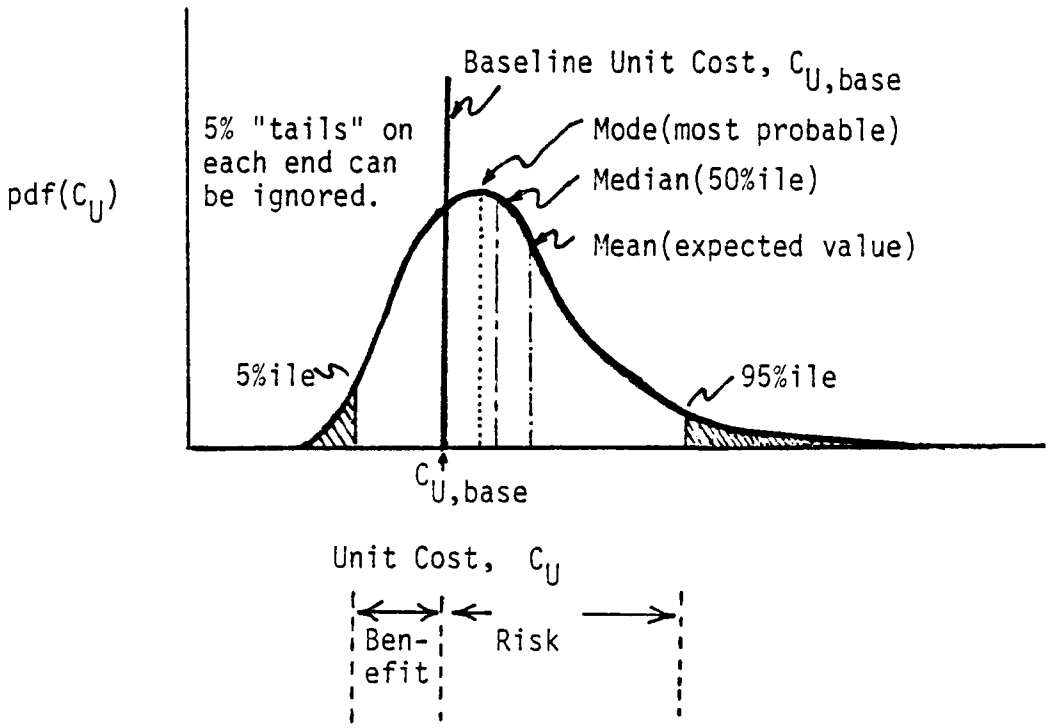


Figure 9.2

Locating a Baseline Unit Cost on a Hypothetical Unit Cost Output Histogram

lower limit to $C_{U,base}$ and assign a probability to attainment of that point. If $C_{U,base}$ lies above (i.e., to the right of) the mode of pdf(C_U), the probability of success is high. This result means that the developer has been very conservative in defining his baseline technology. If $C_{U,base}$ lies to the left or below the mode, one states that the risk is high, i.e., the probability of success is low. In this situation the developer has been overly optimistic in defining his baseline and his future process plant runs a high risk of experiencing unit production costs well over the baseline prediction. When evaluating alternative or competing processes, this type of information is especially useful if the curves and single-point estimates for each process are compared on the same axes. A few scenarios which can occur in such a comparison are analyzed later in this chapter.

The Single Process Decision

For new processes one is faced with the fact that each additional step in the RD&D spectrum will cost considerably more than the previous. In rough terms each step on the scale of RD&D levels I through IV requires an expenditure of funds an order of magnitude higher than the previous step.

For this reason one wishes to gain as much useful economic information as possible prior to the next proceed/do-not-proceed decision. The economic evaluation method described in this document can ascertain for the analyst and developer the cost effects of disappointments in the development program and whether the baseline process was optimistic or pessimistic in light of the prevailing uncertainties.

What is really needed in this determination, however, is a basis for comparison. In many cases alternative, often conventional, processes exist which already produce the same commodity or product. Such is the case with most chemicals and the production of electricity. If a significant fraction of the area beneath the unit cost histogram lies to the right of the unit cost value derived for an existing process, the economic benefits from the new technology are likely to be small and perhaps further development is not warranted. For many processes, however, there are non-economic factors stimulating the development effort, such as environmental benefits, assurance of energy supply, and political considerations.

By conducting periodic economic evaluations in parallel with development, new process baseline and new uncertainty analyses, which incorporate the latest data from the development program, can be compared. After a few such comparisons, and when the predominant development issues driving the economics have been identified, trends should appear that can assist management in making the proceed/do-not-proceed decision. There is no well defined rule or guideline by which decisions of this type can be made. The question often becomes one of how much more capital must the organization spend on development before it really knows whether the process is economic? Many non-technical factors such as the organization's financial position come into this decision.

Evaluation of Competing Processes

This economic assessment methodology is best utilized for the evaluation of alternate or competing processes at a commensurate level of

development and at the same point on the evaluation/cost estimation detail spectrum. When competing processes are considered, a set of "common yardstick" ground rules for evaluation must be set forth. Among the attributes which should be the same for each process are: design or productivity targets, interest rates and other strategic variables, types of figures of merit used, and cost estimating ground rules. If a common site is being considered, other factors such as land costs, labor rates, and utility rates should be the same. Any input variables which are common to two or more processes should have consistent input distributions and ranges.

The problem of comparing processes at differing stages of development is a difficult one at best, especially if the available performance and cost estimates (baselines) are at differing RD&D stages. Application of the figure of merit adjustment factors can compensate somewhat for this problem, when comparing processes in RD&D Levels I and II since the Level I uncertainty evaluation is apt to carry one or more figure-of-merit adjustment factor distributions, and the resulting unit cost distribution for the Level I process analysis will very likely have a wider dispersion or standard deviation. Strategic factors, such as the time value of money must also be considered if the deployment schedules for the processes are markedly different. These should be handled as a separate analysis.

Retrofitted plants, or those in which it is proposed that a conventional step be replaced by a purportedly less expensive novel technology step (Process A in Figure 9.3), can also be analyzed by comparison of distributions. The conventional process (Process B) might have a sharply

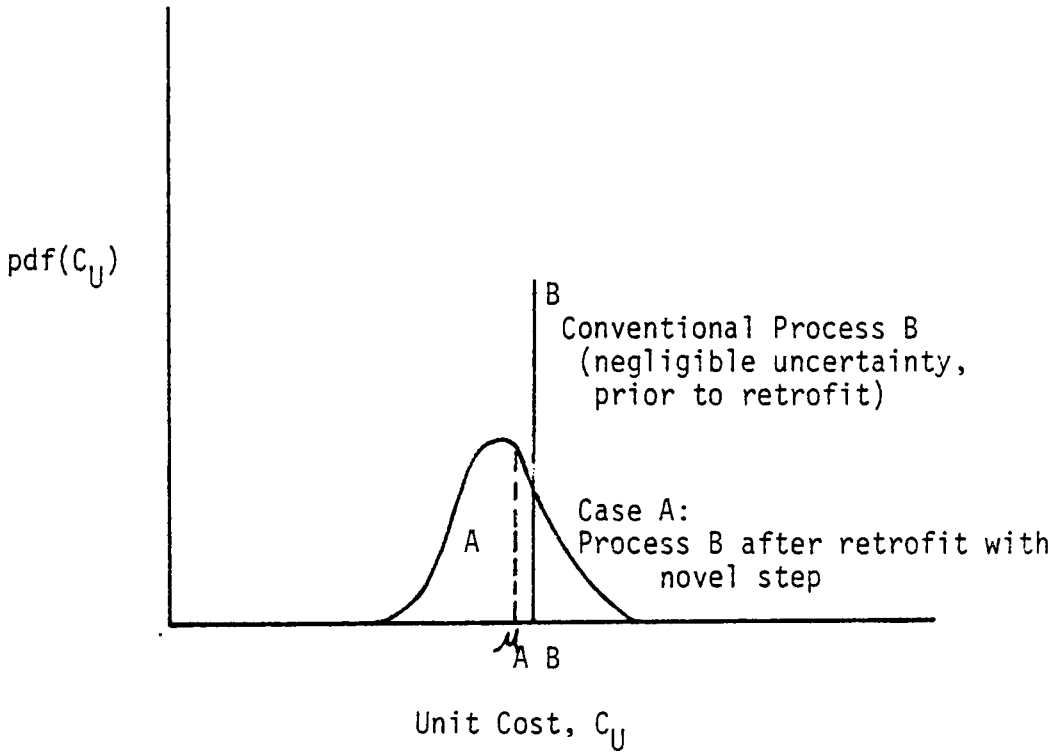


Figure 9.3

Possible Risk Scenario Resulting from Retrofit
of a Novel Step into a Conventional Process

peaked unit cost distribution with little or no uncertainty, whereas addition of a new step will "spread" the distribution and lower the mean unit cost. The area enclosed by the right side tail of the new distribution and the right tail of the conventional process distribution gives some indication of the risk entailed by modifying that process step.

It is of interest to consider a few possible economic risk scenarios and their implications to the decision-maker who must use them. The first plot in Figure 9.4 shows the easiest case for the decision-maker to consider. When plotted on the same figure-of-merit axis, the two output distributions do not overlap. Process A in this case can be said to be 100% certain of attaining a unit cost less than Process B. Based on the process economic risk consideration alone, Process A is a clear winner. From the standpoint of the enterprise, however, the deployment timing of the two processes can be important.

The second plot in Figure 9.4 displays a case where the output distributions overlap but the modes and means of the two distributions still differ significantly. The standard deviations also differ; however, direct comparison of the means of the two distributions is sufficient in this case to justify a clear-cut selection of Process A over Process B. By choosing a desired unit cost, which represents a spike on the cost spectrum, and taking the area to the right of the spike enclosed by each distribution, one can quantitatively assess the economic risk of not attaining the value $C_{U,\text{base des.}}$ The areas to the left of this spike would represent the chance of success.

The third plot in Figure 9.4 considers the more difficult case of two distributions for which the means are close and for which the

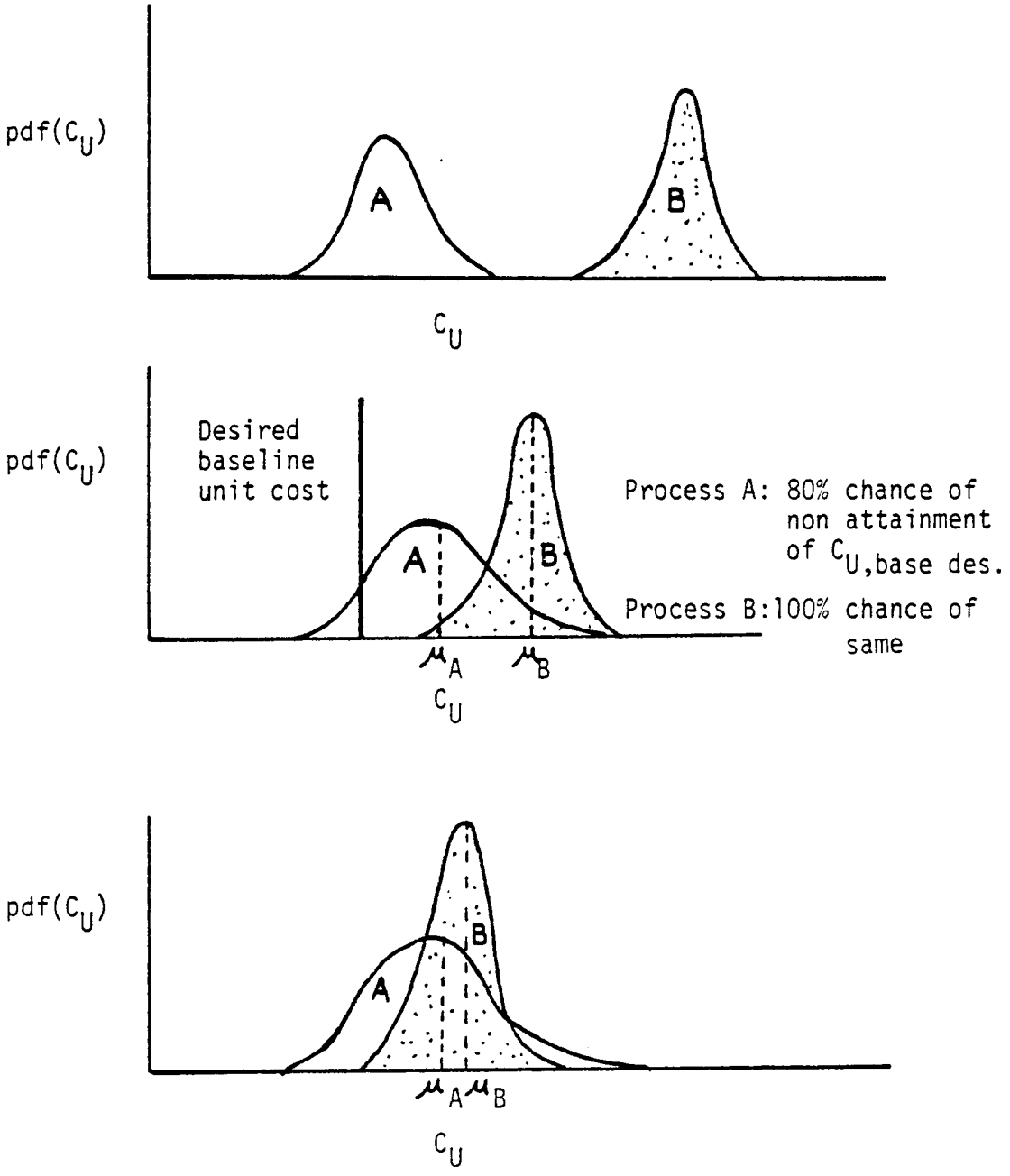


Figure 9.4

Three Risk Scenarios for Comparison
of Two Competing Processes

standard deviations are again somewhat different. Process B has a narrow range, but Process A has some cases included which have much higher costs. When such results are obtained, the decision maker must examine his attitude toward risk and take a harder look at other attributes which might influence a decision. At this point, project management should have available selection criteria which can be consistently applied to each process alternative.

Use in Conjunction With Selection Criteria

A scoring or weighting system can be developed to accompany a set of selection criteria. These criteria and other evaluation models (task I and task III) can be used to augment this quantitative method of economic assessment as part of an overall selection procedure. Among other categories not included in the above economic assessment methodology but worthy of consideration are:

1. Benefit/Risk: In addition to economic or cost risk, the developer should consider the financial benefit of a project to the overall enterprise for a particular firm or government program. The distributions from the risk model above can be input to a separate DCF type program more typical of the financial analysis applications suggested by Hertz. Figures of merit can be invented for use as indicators of benefit/risk.

2. Program Management Plans: Not all organizations are equally competent at developing and commercializing high technology energy projects. One needs to consider the competence and experience of the management and development teams, program planning documents, and the

contractor's or firm's past histories in bringing projects from the R&D stage to the production plant stage.

3. Adequacy of Baseline Engineering Designs: This category should not rate the adequacy of the engineering design and cost scaling part of the process model, rather it should rate the inclusiveness, clarity, reasonableness, and presentation of the most current baseline plant design and cost estimates performed by an engineering team and made available by the process proponent. In many instances different engineering teams of varying abilities may have prepared each estimate. The competence of each team will be reflected in its design documents.

4. Adequacy of Proposed Large-Scale Demonstration Facility Designs: This category rates the same attributes as 3. above except that the proposed pilot plant or proposed large-scale demonstration facility engineering design and cost estimates are rated. For some processes, especially those in RD&D Stages I and II, these data may not exist.

The weighting of all categories, including the data base resulting from the economic evaluation results, is subjective and personal attitudes toward the importance of various project attributes are important. Individual firms historically may place emphasis on different areas. A high-technology aerospace firm may be less concerned with risk and more concerned with management style, whereas a conservative chemical company might be concerned primarily with project economic benefit. The case of whether the project is privately or publically funded also weighs heavily in their relative weightings. Governments often have the mission of taking on high-risk RD&D with payoff in the distant future. Private enterprise generally orients RD&D programs toward short-term profit

goals. These differing attitudes toward risk are important and comprise a discipline of their own known as utility theory.

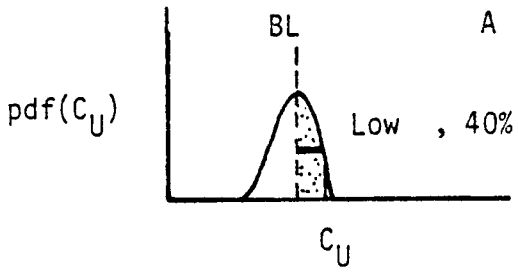
Conditional Multi-Variable Sensitivity Studies

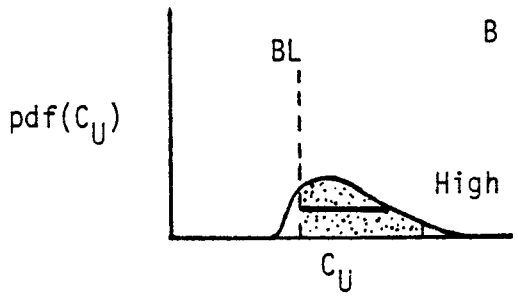
Other Uses of MVSS in Process Evaluation

One can utilize the previous techniques to investigate the sensitivity effects of submitting selected smaller generic groups of input variables rather than submitting all possible input variables available to the ensemble. Such "conditional sensitivity studies" require setting all variables which are not of interest to their mode (or baseline) values and simultaneously varying the inputs which represent the generic category of interest to the analyst. By this method, one can separate hardware cost uncertainty effects from performance uncertainty effects, capital cost uncertainties from operating cost uncertainties, and the uncertainty arising from one process step or subsystem from the uncertainty in other process steps. For each case representing a partial ensemble the standard deviation of the resultant output distribution or the output pdf area above the predicted baseline will give some indication of the relative sensitivity of the unit cost to that generic category of variables. Figure 9.5 shows a typical breakdown resulting from partitioning of MVSS input ensembles in this manner. A fictitious 10 input variable model is assumed to exist for this example.

Comparison of Processes with Different Deployment Schedules

The time value of money dictates that increased benefit can be derived from an economically attractive process that is brought into





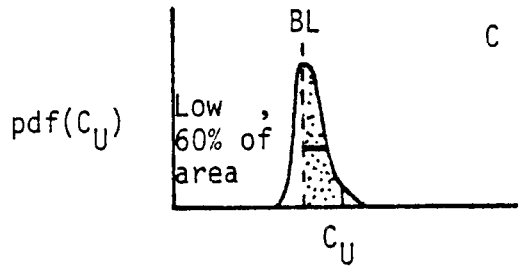
CONDITIONAL MVSS's
10 Total Input (X_i)Variables

Case A: Vary X_1 & X_2 only

Case B: Vary all X_i, X_1-X_{10}

Case C: Vary X_5,X_6 & X_7 only

Case D: Vary X_3, X_8,X_9,X_{10}



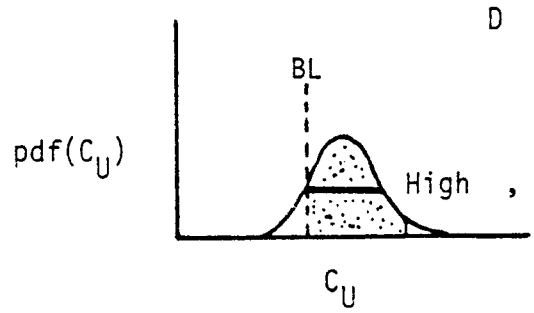


Figure 9.5

Results Generated by a Typical Conditional
Multi-Variable Sensitivity Study

production sooner as opposed to another process with the same projected unit cost that is brought into production later. The unit cost, as presented in Chapter VI, is not an adequate figure of merit for handling this situation nor is the methodology described here designed to answer such strategic questions.

To initiate such a strategic modeling effort the analyst must now convert capital and operating costs into yearly cash flows which can be present valued. This requires development of a construction and production schedule for each process. Such schedules will themselves be subject to considerable uncertainty. The effect of schedule uncertainty on the net present worth can be calculated via a simple DCF model and application of the Monte Carlo technique. For this schedule uncertainty analysis (task III), it is best to set the technology and cost variables at fixed values and not attempt to mix technological and schedule uncertainties. By treating each separately the analyst can better separate the causal relationships. Economics models can exist separately from process assessment models when one can make the assumption that optimization of the technology is independent of the details of deployment.

SVSS Results for the XYZ Process

Up to this point, the only uncertain input variables considered in the XYZ example was the catalyst activity, k. The method of single variable sensitivity studies (SVSS) described in Chapter VIII can be used to search for other input variables with high economic leverage. Figure 9.6 shows how SVSS was used to determine that the unit feed cost for compound "A" (CFO) and the unit cost of catalyst (CCAT) were also

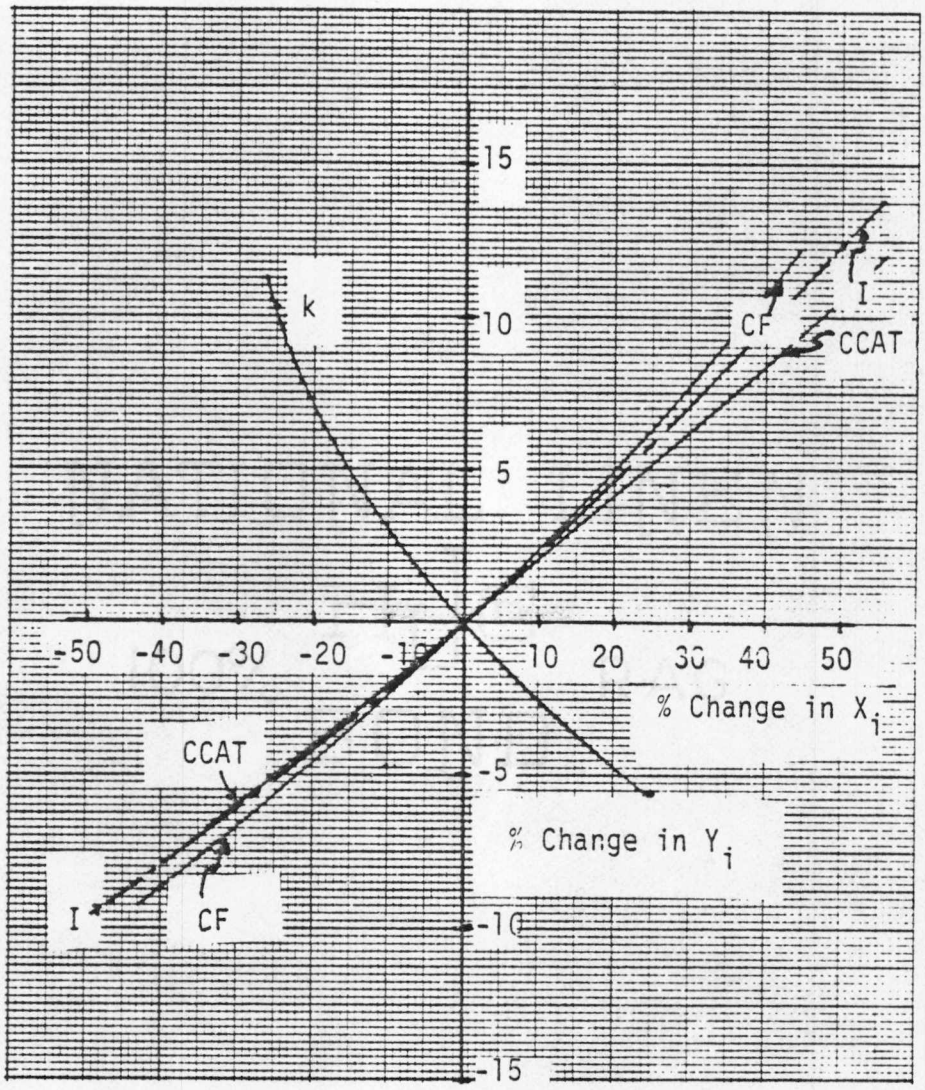


Figure 9.6

Single Value Sensitivity Study Including Effect of Interest Rate, I, for XYZ Process

significant economic drivers. The catalyst activity, k, shows the largest absolute value for its slope about the baseline case (origin), hence it represents the strongest drivers of the unit costs. The optimizing model (Appendix H) with the revised cost scaling algorithms was used to generate these results.

A Three Variable Monte Carlo Simulation for the XYZ Process

Using the three part FORTRAN model shown as an example in Appendix H and the three input variables identified above, an example simulation will now be shown. It is presumed that the economic analysts and developers of the XYZ catalyst have held a peer review session in which the model and the inputs have undergone critical analysis. The "best-guess," and in this case most-likely (mode), values for the three input variables of importance are shown in Figure 9.7 along with their pdf's. Figure 9.8 shows the 1,000 iteration output histograms which result for the input variables, several internal variables, and most importantly the unit cost figure of merit.

As expected a bell-shaped curve results, in this case skewed somewhat toward higher unit cost values. The reason for the skewness is discussed in the next chapter. Table 9.1 summarizes the statistical parameters for the example unit cost distributions.

Application of Methodology to Photochemical Syngas Cleanup Process: Results and Interpretation

Interpretation of Simulation Histograms and Statistics

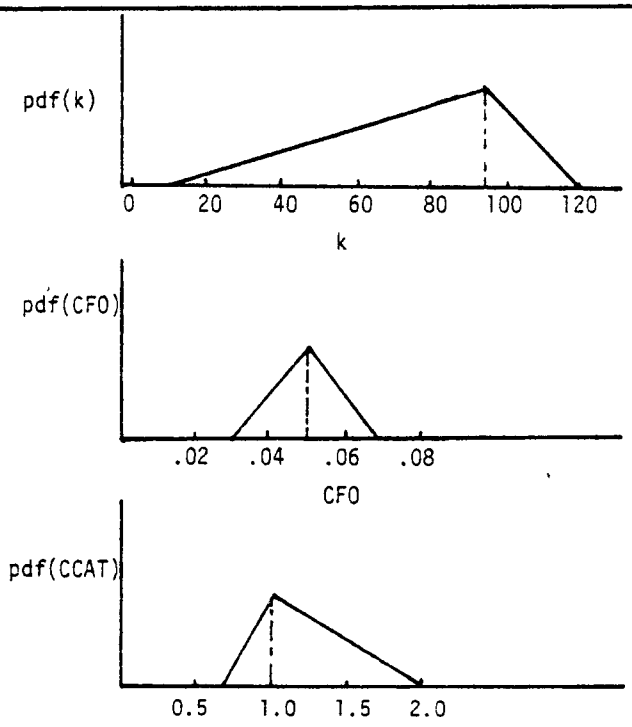
Figure 9.9 shows a histogram representing a probability density function for an output figure of merit, in this case the unit production

MONTE CARLO UNCERTAINTY ANALYSIS FOR XYZ CASE
DATE: TIME: 09:48

3 INPUT VARIABLES 6 OUTPUT VARIABLES 1000 ITERATIONS
9 STORAGE LOCATIONS USED FOR INPUT DATA

SUMMARY OF INPUT DATA

I	NAME	DIST	DATA		
			Mode	Low	High
1	K	TRIANGLE	96.00	12.00	120.0
2	CF0	TRIANGLE	0.5000E-01	0.3000E-01	0.7000E-01
3	CCAT	TRIANGLE	1.000	0.7000	2.000




```
# of   # of
inputs outputs (Actual data set for simulation)
  0306  1000XYZ CASE
  -1K       96.       12.       120.
  -1CF0     0.05      0.03      0.07
  -1CCAT    1.        .7        2.
  XA0     P0      V       CTOTS   COP     CUNIT
```

Figure 9.7

MVSS Inputs for XYZ Process Simulation

STATISTICS FOR INPUT VARIABLE K (Reaction Rate Constant with XYZ Catalyst, liters fluid/(hr-liter catalyst))

MINIMUM 12.757 MAXIMUM 119.52

MEAN 76.429 VARIANCE 561.07 STD.DEVIATION 23.687

PERCENTILES: 2.5% 26.0 5.0% 32.5 50.0% 80.5 95.0% 110. 97.5% 113.

1000 POINT HISTOGRAM * = 2 POINTS

PROB	CUME	VALUE		
0.0010	0.0000	10.00	1	*
0.0050	0.0010	15.00	5	***
0.0160	0.0060	20.00	16	********
0.0150	0.0220	25.00	15	********
0.0260	0.0370	30.00	26	*************
0.0310	0.0630	35.00	31	*****************
0.0330	0.0940	40.00	33	******************
0.0370	0.1270	45.00	37	********************
0.0370	0.1640	50.00	37	********************
0.0560	0.2010	55.00	56	*****************************
0.0500	0.2570	60.00	50	*************************
0.0570	0.3070	65.00	57	*****************************
0.0640	0.3640	70.00	64	********************************
0.0640	0.4280	75.00	64	********************************
0.0830	0.4920	80.00	83	***
0.0830	0.5750	85.00	83	***
0.0950	0.6580	90.00	95	**
0.0800	0.7530	95.00	80	**
0.0710	0.8330	100.0	71	***********************************
0.0480	0.9040	105.0	48	************************
0.0350	0.9520	110.0	35	******************
0.0130	0.9870	115.0	13	*******
	1.0000	120.0		

Figure 9.8

Histograms Resulting from XYZ Process Simulation

STATISTICS FOR INPUT VARIABLE CF0 (Unit Cost of Feedstock "A", $/g-mol)

MINIMUM 3.04111E-02 MAXIMUM 6.99465E-02

MEAN 5.00131E-02 VARIANCE 7.00998E-05 STD.DEVIATION 8.37256E-03

PERCENTILES: 2.5%3.435E-02 5.0%3.582E-02 50.0%5.004E-02 95.0%6.414E-02 97.5%6.586E-02

1000 POINT HISTOGRAM * = 2 POINTS

PROB	CUME	VALUE		
0.0060	0.0000	3.0000E-02	6	***
0.0130	0.0060	3.2000E-02	13	*******
0.0340	0.0190	3.4000E-02	34	*****************
0.0350	0.0530	3.6000E-02	35	*****************
0.0410	0.0880	3.8000E-02	41	********************
0.0670	0.1290	4.0000E-02	67	**********************************
0.0560	0.1960	4.2000E-02	56	****************************
0.0750	0.2520	4.4000E-02	75	**************************************
0.0830	0.3270	4.6000E-02	83	**
0.0880	0.4100	4.8000E-02	88	**
0.0940	0.4980	5.0000E-02	94	**
0.0890	0.5920	5.2000E-02	89	**
0.0680	0.6810	5.4000E-02	68	**********************************
0.0640	0.7490	5.6000E-02	64	********************************
0.0510	0.8130	5.8000E-02	51	*************************
0.0540	0.8640	6.0000E-02	54	***************************
0.0300	0.9180	6.2000E-02	30	***************
0.0290	0.9480	6.4000E-02	29	***************
0.0140	0.9770	6.6000E-02	14	*******
0.0090	0.9910	6.8000E-02	9	*****
	1.0000	7.0000E-02		

Figure 9.8 (Continued)

STATISTICS FOR INPUT VARIABLE CCAT (Unit Cost of XYZ Catalyst, $/gram)

MINIMUM 0.71348 MAXIMUM 1.9785

MEAN 1.2272 VARIANCE 7.58931E-02 STD.DEVIATION 0.27549

PERCENTILES: 2.5% .797 5.0% .848 50.0% 1.19 95.0% 1.77 97.5% 1.83

1000 POINT HISTOGRAM * = 1 POINTS

PROB	CUME	VALUE		
0.0070	0.0000	0.7000	7	*******
0.0190	0.0070	0.7500	19	*******************
0.0250	0.0260	0.8000	25	*************************
0.0490	0.0510	0.8500	49	***
0.0630	0.1000	0.9000	63	***
0.0720	0.1630	0.9500	72	**
0.0730	0.2350	1.000	73	***
0.0700	0.3080	1.050	70	**
0.0660	0.3780	1.100	66	**
0.0740	0.4440	1.150	74	**
0.0580	0.5180	1.200	58	**
0.0610	0.5760	1.250	61	***
0.0540	0.6370	1.300	54	**
0.0530	0.6910	1.350	53	***
0.0510	0.7440	1.400	51	***
0.0330	0.7950	1.450	33	**********************************
0.0320	0.8280	1.500	32	*********************************
0.0320	0.8600	1.550	32	*********************************
0.0180	0.8920	1.600	18	******************
0.0160	0.9100	1.650	16	****************
0.0150	0.9260	1.700	15	***************
0.0230	0.9410	1.750	23	************************
0.0160	0.9640	1.800	16	****************
0.0090	0.9800	1.850	9	*********
0.0070	0.9890	1.900	7	*******
0.0040	0.9960	1.950	4	****
	1.0000	2.000		

Figure 9.8 (Continued)

1000 POINT HISTOGRAM * = 3 POINTS

PROB	CUME	VALUE		
0.0010	0.0000	160.0	1	
0.0270	0.0010	180.0	27	*********
0.1180	0.0280	200.0	118	**
0.1610	0.1460	220.0	161	**
0.1600	0.3070	240.0	160	***
0.1120	0.4670	260.0	112	**************************************
0.0880	0.5790	280.0	88	******************************
0.0630	0.6670	300.0	63	**********************
0.0540	0.7300	320.0	54	*******************
0.0420	0.7840	340.0	42	***************
0.0240	0.8260	360.0	24	********
0.0220	0.8500	380.0	22	*******
0.0210	0.8720	400.0	21	*******
0.0250	0.8930	420.0	25	********
0.0160	0.9180	440.0	16	*****
0.0120	0.9340	460.0	12	****
0.0010	0.9460	480.0	1	
0.0060	0.9470	500.0	6	**
0.0080	0.9530	520.0	8	***
0.0050	0.9610	540.0	5	**
0.0040	0.9660	560.0	4	*
0.0040	0.9700	580.0	4	*
0.0060	0.9740	600.0	6	**
0.0030	0.9800	620.0	3	*
0.0030	0.9830	640.0	3	*
0.0030	0.9860	660.0	3	*
0.0020	0.9890	680.0	2	*
0.0000	0.9910	700.0	0	
0.0020	0.9910	720.0	2	*
0.0000	0.9930	740.0	0	
0.0010	0.9930	760.0	1	
0.0000	0.9940	780.0	0	
0.0020	0.9940	800.0	2	*
0.0010	0.9960	820.0	1	
0.0010	0.9970	840.0	1	
0.0010	0.9980	860.0	1	
	0.9990	880.0		

STATISTICS FOR OUTPUT VARIABLE V (Plug Flow Reactor Volume, liters)

MINIMUM 177.18 MAXIMUM 1055.3

MEAN 297.85 VARIANCE 10602. STD.DEVIATION 102.97

PERCENTILES: 2.5% 198. 5.0% 204. 50.0% 266. 95.0% 510.

97.5% 603.

Figure 9.8 (Continued)

STATISTICS FOR OUTPUT VARIABLE XA0 (Conversion of "A" to "R")

MINIMUM 0.35000 MAXIMUM 0.70000

MEAN 0.56837 VARIANCE 4.06727E-03 STD.DEVIATION 6.37752E-02

PERCENTILES: 2.5% .421 5.0% .443 50.0% .575 95.0% .650 97.5% .659

1000 POINT HISTOGRAM * = 3 POINTS

PROB	CUME	VALUE		
0.0050	0.0000	0.3500	5	**
0.0000	0.0050	0.3600	0	
0.0000	0.0050	0.3700	0	
0.0000	0.0050	0.3800	0	
0.0140	0.0050	0.3900	14	*****
0.0030	0.0190	0.4000	3	*
0.0000	0.0220	0.4100	0	
0.0230	0.0220	0.4200	23	********
0.0000	0.0450	0.4300	0	
0.0160	0.0450	0.4400	16	*****
0.0000	0.0610	0.4500	0	
0.0520	0.0610	0.4600	52	******************
0.0000	0.1130	0.4700	0	
0.0330	0.1130	0.4800	33	***********
0.0190	0.1460	0.4900	19	******
0.0310	0.1650	0.5000	31	**********
0.0000	0.1960	0.5100	0	
0.0000	0.1960	0.5200	0	
0.1230	0.1960	0.5300	123	**
0.0560	0.3190	0.5400	56	*******************
0.0000	0.3750	0.5500	0	
0.0570	0.3750	0.5600	57	*******************
0.1250	0.4320	0.5700	125	**
0.0000	0.5570	0.5800	0	
0.0000	0.5570	0.5900	0	
0.2090	0.5570	0.6000	209	**********
0.0760	0.7660	0.6100	76	*************************
0.0000	0.8420	0.6200	0	
0.0000	0.8420	0.6300	0	
0.1100	0.8420	0.6400	110	************************************
0.0250	0.9520	0.6500	25	********
0.0000	0.9770	0.6600	0	
0.0110	0.9770	0.6700	11	****
0.0090	0.9880	0.6800	9	***
0.0000	0.9970	0.6900	0	
0.0030	0.9970	0.7000	3	*
	1.0000	0.7100		

Figure 9.8 (Continued)

STATISTICS FOR OUTPUT VARIABLE P0 (Productivity, g-mol of "R" per hour)

MINIMUM 2800.0 MAXIMUM 2800.0

MEAN 2800.0 VARIANCE 0.00000E+00 STD.DEVIATION 0.00000E+00

PERCENTILES: 2.5%2.803E+03 5.0%2.805E+03 50.0%2.850E+03 95.0%2.895E+03 97.5%2.898E+03

1000 POINT HISTOGRAM * = 14 POINTS

PROB	CUME	VALUE		
0.0000	0.0000	0.0000E+00	0	
0.0000	0.0000	100.0	0	
0.0000	0.0000	200.0	0	
0.0000	0.0000	300.0	0	
0.0000	0.0000	400.0	0	
0.0000	0.0000	500.0	0	
0.0000	0.0000	600.0	0	
0.0000	0.0000	700.0	0	
0.0000	0.0000	800.0	0	
0.0000	0.0000	900.0	0	
0.0000	0.0000	1000.	0	
0.0000	0.0000	1100.	0	
0.0000	0.0000	1200.	0	
0.0000	0.0000	1300.	0	
0.0000	0.0000	1400.	0	
0.0000	0.0000	1500.	0	
0.0000	0.0000	1600.	0	
0.0000	0.0000	1700.	0	
0.0000	0.0000	1800.	0	
0.0000	0.0000	1900.	0	
0.0000	0.0000	2000.	0	
0.0000	0.0000	2100.	0	
0.0000	0.0000	2200.	0	
0.0000	0.0000	2300.	0	
0.0000	0.0000	2400.	0	
0.0000	0.0000	2500.	0	
0.0000	0.0000	2600.	0	
0.0000	0.0000	2700.	0	
1.0000	0.0000	2800.	1000	**********
	1.0000	2900.		

Figure 9.8 (Continued)

STATISTICS FOR OUTPUT VARIABLE CTOTS(Total Capital Cost for XYZ Process)

MINIMUM 3.51351E+06 MAXIMUM 1.67628E+07

MEAN 5.70855E+06 VARIANCE 3.01845E+12 STD.DEVIATION 1.73737E+06

PERCENTILES: 2.5%3.702E+06 5.0%3.903E+06 50.0%5.250E+06 95.0%9.154E+06 97.5%1.067E+07

1000 POINT HISTOGRAM * = 3 POINTS

PROB	CUME	VALUE		
0.0620	0.0000	3.5000E+06	62	**********
0.1560	0.0620	4.0000E+06	156	**********
0.2000	0.2180	4.5000E+06	200	**********
0.1640	0.4180	5.0000E+06	164	**********
0.1310	0.5820	5.5000E+06	131	**********
0.0700	0.7130	6.0000E+06	70	**********
0.0510	0.7830	6.5000E+06	51	**********
0.0480	0.8340	7.0000E+06	48	**********
0.0210	0.8820	7.5000E+06	21	*******
0.0180	0.9030	8.0000E+06	18	******
0.0250	0.9210	8.5000E+06	25	********
0.0130	0.9460	9.0000E+06	13	****
0.0070	0.9590	9.5000E+06	7	**
0.0070	0.9660	1.0000E+07	7	**
0.0060	0.9730	1.0500E+07	6	**
0.0060	0.9790	1.1000E+07	6	**
0.0050	0.9850	1.1500E+07	5	**
0.0030	0.9900	1.2000E+07	3	*
0.0000	0.9930	1.2500E+07	0	
0.0010	0.9930	1.3000E+07	1	
0.0010	0.9940	1.3500E+07	1	
0.0020	0.9950	1.4000E+07	2	*
0.0010	0.9970	1.4500E+07	1	
0.0010	0.9980	1.5000E+07	1	
0.0000	0.9990	1.5500E+07	0	
0.0000	0.9990	1.6000E+07	0	
0.0010	0.9990	1.6500E+07	1	
	1.0000	1.7000E+07		

Figure 9.8 (Continued)

STATISTICS FOR OUTPUT VARIABLE COP (Total Annual Operating Costs, $/yr)

MINIMUM 1.22398E+06 MAXIMUM 2.60738E+06

MEAN 1.58836E+06 VARIANCE 3.89382E+10 STD.DEVIATION 1.97328E+05

PERCENTILES: 2.5%1.311E+06 5.0%1.341E+06 50.0%1.548E+06 95.0%1.980E+06 97.5%2.114E+06

1000 POINT HISTOGRAM * = 2 POINTS

PROB	CUME	VALUE		
0.0020	0.0000	1.2000E+06	2	*
0.0140	0.0020	1.2500E+06	14	*******
0.0410	0.0160	1.3000E+06	41	*********************
0.0680	0.0570	1.3500E+06	68	**********************************
0.1130	0.1250	1.4000E+06	113	**********
0.1170	0.2380	1.4500E+06	117	**********
0.1500	0.3550	1.5000E+06	150	**********
0.1180	0.5050	1.5500E+06	118	**********
0.0960	0.6230	1.6000E+06	96	**********
0.0580	0.7190	1.6500E+06	58	**********
0.0520	0.7770	1.7000E+06	52	**********
0.0430	0.8290	1.7500E+06	43	**********
0.0330	0.8720	1.8000E+06	33	**********
0.0200	0.9050	1.8500E+06	20	**********
0.0160	0.9250	1.9000E+06	16	********
0.0150	0.9410	1.9500E+06	15	********
0.0110	0.9560	2.0000E+06	11	******
0.0060	0.9670	2.0500E+06	6	***
0.0070	0.9730	2.1000E+06	7	****
0.0040	0.9800	2.1500E+06	4	**
0.0040	0.9840	2.2000E+06	4	**
0.0010	0.9880	2.2500E+06	1	*
0.0060	0.9890	2.3000E+06	6	***
0.0020	0.9950	2.3500E+06	2	*
0.0010	0.9970	2.4000E+06	1	*
0.0010	0.9980	2.4500E+06	1	*
0.0000	0.9990	2.5000E+06	0	
0.0000	0.9990	2.5500E+06	0	
0.0010	0.9990	2.6000E+06	1	*
	1.0000	2.6500E+06		

Figure 9.8 (Continued)

STATISTICS FOR OUTPUT VARIABLE CUNIT (Unit Cost of Product "R", $/gm-mol)

MINIMUM 7.37086E-02 MAXIMUM 0.21103

MEAN 0.10263 VARIANCE 3.76263E-04 STD.DEVIATION 1.93975E-02

PERCENTILES: 2.5% 7.850E-02 5.0% 8.087E-02 50.0% 9.789E-02 95.0% .141 97.5% .157

1000 POINT HISTOGRAM * = 3 POINTS

PROB	CUME	VALUE		
0.0040	0.0000	7.0000E-02	4	*
0.0300	0.0040	7.5000E-02	30	**********
0.0920	0.0340	8.0000E-02	92	*******************************
0.1230	0.1260	8.5000E-02	123	***
0.1700	0.2490	9.0000E-02	170	**
0.1400	0.4190	9.5000E-02	140	**
0.1200	0.5590	0.1000	120	***
0.0830	0.6790	0.1050	83	****************************
0.0480	0.7620	0.1100	48	****************
0.0450	0.8100	0.1150	45	***************
0.0350	0.8550	0.1200	35	************
0.0180	0.8900	0.1250	18	******
0.0220	0.9080	0.1300	22	*******
0.0170	0.9300	0.1350	17	******
0.0120	0.9470	0.1400	12	****
0.0090	0.9590	0.1450	9	***
0.0040	0.9680	0.1500	4	*
0.0070	0.9720	0.1550	7	**
0.0060	0.9790	0.1600	6	**
0.0020	0.9850	0.1650	2	*
0.0040	0.9870	0.1700	4	*
0.0020	0.9910	0.1750	2	*
0.0000	0.9930	0.1800	0	
0.0020	0.9930	0.1850	2	*
0.0030	0.9950	0.1900	3	*
0.0000	0.9980	0.1950	0	
0.0000	0.9980	0.2000	0	
0.0010	0.9980	0.2050	1	
0.0010	0.9990	0.2100	1	
	1.0000	0.2150		

Figure 9.8 (Continued)

Table 9.1

Statistics for Figures of Merit Generated in XYZ Process Simulation

Baseline	Figure of Merit	5 Percentile	Median 50 Percentile	95 Percentile	Mode Range	Mean	Standard Deviation
4.32	Total Capital Cost ($MM)	3.90	5.25	9.15	4.5-5.0	5.71	1.73
2.103	Total Annual ($MM)	1.34	1.55	1.98	1.5-1.55	1.59	0.20
.0858	Unit Cost of Production ($/gmol R)	0.0809	0.0979	0.141	0.085-0.090	0.1026	0.019

500 POINT HISTOGRAM * = 1 POINTS

PROB	CUME	VALUE		
0.0300	0.0000	190.0	15	***************
0.1320	0.0300	195.0	66	**********
0.1200	0.1620	200.0	60	**********
0.1240	0.2820	205.0	62	**********
0.1000	0.4060	210.0	50	**********
0.0800	0.5060	215.0	40	**********
0.0780	0.5860	220.0	39	**********
0.0480	0.6640	225.0	24	**********
0.0420	0.7120	230.0	21	**********
0.0360	0.7540	235.0	18	**********
0.0340	0.7900	240.0	17	**********
0.0200	0.8240	245.0	10	**********
0.0140	0.8440	250.0	7	*******
0.0200	0.8580	255.0	10	**********
0.0120	0.8780	260.0	6	******
0.0120	0.8900	265.0	6	******
0.0040	0.9020	270.0	2	**
0.0140	0.9060	275.0	7	*******
0.0060	0.9200	280.0	3	***
0.0080	0.9260	285.0	4	****
0.0040	0.9340	290.0	2	**
0.0060	0.9380	295.0	3	***
0.0040	0.9440	300.0	2	**
0.0140	0.9480	305.0	7	*******
0.0000	0.9620	310.0	0	
0.0060	0.9620	315.0	3	***
0.0040	0.9680	320.0	2	**
0.0000	0.9720	325.0	0	
0.0000	0.9720	330.0	0	
0.0020	0.9720	335.0	1	*
0.0040	0.9740	340.0	2	**
0.0040	0.9780	345.0	2	**
0.0000	0.9820	350.0	0	
0.0000	0.9820	355.0	0	
0.0020	0.9820	360.0	1	*
0.0000	0.9840	365.0	0	
0.0000	0.9840	370.0	0	
0.0020	0.9840	375.0	1	*
	0.9860	380.0		

~ Baseline Unit Cost

MVSS #1: 12 Input Variables

STATISTICS FOR OUTPUT VARIABLE TON

(Unit Cost of Methanol Produced by Catalytic Process
Which Includes Photochemical S Removal, $/ton MeOH)

MINIMUM 190.69 MAXIMUM 495.19

MEAN 226.89 VARIANCE 1556.1 STD.DEVIATION 39.448

PERCENTILES: 2.5% 194. 5.0% 196. 50.0% 215. 95.0% 306.
97.5% 340.

Figure 9.9

Simulation Result for Photochemical Syngas Cleanup Process

cost ($/ton) of methanol with a photolytic sulfur removal system. The assessment model for this process is discussed in Appendix I and the FORTRAN code listing is in Appendix J. Twelve uncertain input variables were included in this MVSS. No figure-of-merit adjustment factors were included in this example. As expected a positively skewed bell-shaped histogram appears. Each asterisk (*) represents one case appearing in a particular cost bin where each bin has a range of $5 per ton. The values of the pdf and cdf are tabulated along with the number of cases appearing in each bin. A total of 500 cases or iterations was generated. As would be expected in a new process of this sort, the output histogram is skewed toward higher unit costs. A few cases fall in a very high range ($300+ per ton) and are cases in which most of all the inputs assumed adverse values. In order to prevent overemphasis of such maximum (or minimum) or long tail values, it is prudent to report the middle 90%. These are the values lying between the 5 percentile and 95 percentile. In this case this would be the range from $196 to $306 per ton. The most probable or mode value can only be represented with the accuracy of the width of a bin, i.e., one can say that the methanol cost will most likely between $195 to $200 per ton, i.e., the second bin. The mean or expected value is calculated as $227 per ton. The standard deviation is useful for indicating the extent to which the results are dispersed about the mean. Table 2.1 in Chapter II summarized the standard deviation and other statistical parameters for this case.

It should be noted that a curve drawn along the tops of each histogram segment will not be smooth and that some bins in the tails region are even empty. Part of this behavior is due to poor statistics i.e., too few iterations. Most of the unevenness, however, is due to discontinuities within the code itself. Many hardware cost items, such as compressors or lasers must be counted as discrete items, hence, the resulting cost functions have a step-like appearance.

Relationship of Uncertainty Results to the Base Case

A single point methanol cost of $200.8 per ton was estimated for the baseline photolytic syngas cleanup process (Data in Appendix K) and its location on the uncertainty histogram is shown on Fig 9.9. The uncertainty analysis used triangular pdf mode values somewhat more pessimistic than baseline for only two of the twelve important input variables. Selections of the actual MVSS inputs for this example is discussed in Appendix I.

Results similar to those above have been obtained in analyses of other new processes, specifically those for advanced isotope separation. Chapter X will discuss the conclusions drawn from these and the above (photochemical process) application of this methodology.

CHAPTER X

CONCLUSIONS AND PERTINENT OBSERVATIONS CONCERNING USE OF THE METHODOLOGY

Major Conclusions

The application and use of this methodology for the economic evaluation of new uranium enrichment processes and the photochemical process discussed in Appendix I have allowed the author to draw two major conclusions and several less global observations. Since the XYZ example was a purely fictitious process and only meant a simple illustration of the methodology, no historical conclusions relative to use of this methodology were drawn from its use as an example.

The two major conclusions deal with the analysis and comparison of figure of merit uncertainty ranges generated by the Monte Carlo technique with the process proponent's "best-guess" figure of merit value.

First Conclusion

For processes in the early R&D stages, uncertainty in process productivity or performance, rather than the uncertainty in process hardware costs, causes the largest variance in the output unit cost figure of merit. By conditional MVSS methods the hardware cost related input variables (such as $/watt of laser power and equipment MTBFs for the photochemical process in Appendix I) were submitted to an MVSS in which performance related variables (such as cross sections and rate coefficients) were held constant. A conditional MVSS for the converse situation was also performed. For all processes evaluated (the AIS pro-

cesses and the photolytic syngas cleanup process in Appendix I), the variance (or middle 90% range for the unit cost) obtained from the input of uncertain performance variables greatly exceeded the variance or range obtained from running hardware cost input alone. Figure 10.1 shows the two conditional MVSS output histograms for the photochemical process discussed in Appendix I. The total MVSS (all 12 variables uncertain) is shown in Figure 9.9. Uncertainty in performance inputs generated a middle 90% unit cost range of $196/ton MeOH to $295/ton MeOH, and uncertainty in hardware cost inputs generated a middle 90% range of $201/ton MeOH to $209/ton MeOH. Table 2.1 in Chapter II summarizes these results.

In general it has been shown that early in the R&D program one can estimate hardware costs (for an assumed performance) much better than one can estimate the performance by itself. Assurance that predicted performance can indeed be reached should be the major goal of R&D in the early stages. Hardware costs and strategic questions should not be ignored; however, performance is essentially what "makes or breaks" the process; therefore, its attainment should require first priority in the development program.

Second conclusion. Upon completion of an analysis of uncertainty, the process proponent's baseline or "best-guess" unit cost often falls on the low (optimistic) end of the output unit cost frequency histogram. It is perhaps not surprising that a development proponent will choose a somewhat optimistic baseline case. The developer must often compete for funding with other projects and always wants to present the best reasonable prediction. Experience has shown, however, that such optimistic baselines often rest on inadequate models used in the development program

500 POINT HISTOGRAM * = 1 POINTS

Fig. of Merit TON is Unit Cost of Methanol in $/ton

PROB	CUME	VALUE		
0.0320	0.0000	190.0	16	****************
0.1420	0.0320	195.0	71	**********
0.1300	0.1740	200.0	65	**********
0.1340	0.3040	205.0	67	**********
0.1180	0.4380	210.0	59	**********
0.0720	0.5560	215.0	36	**********
0.0680	0.6280	220.0	34	**********
0.0460	0.6960	225.0	23	**********
0.0300	0.7420	230.0	15	**********
0.0320	0.7720	235.0	16	**********
0.0320	0.8040	240.0	16	**********
0.0260	0.8360	245.0	13	**********
0.0140	0.8620	250.0	7	*******
0.0180	0.8760	255.0	9	*********
0.0080	0.8940	260.0	4	****
0.0100	0.9020	265.0	5	*****
0.0120	0.9120	270.0	6	******
0.0080	0.9240	275.0	4	****
0.0040	0.9320	280.0	2	**
0.0060	0.9360	285.0	3	***
0.0080	0.9420	290.0	4	****
0.0080	0.9500	295.0	4	****
0.0040	0.9580	300.0	2	**
0.0060	0.9620	305.0	3	***
0.0060	0.9680	310.0	3	***
0.0020	0.9740	315.0	1	*
0.0020	0.9760	320.0	1	*
0.0020	0.9780	325.0	1	*
0.0000	0.9800	330.0	0	
0.0020	0.9800	335.0	1	*
0.0000	0.9820	340.0	0	
0.0000	0.9820	345.0	0	
0.0000	0.9820	350.0	0	
0.0020	0.9820	355.0	1	*
0.0020	0.9840	360.0	1	*
0.0000	0.9860	365.0	0	
0.0020	0.9860	370.0	1	*
0.0000	0.9880	375.0	0	
0.0000	0.9880	380.0	0	
0.0020	0.9880	385.0	1	*
	0.9900	390.0		

BL bin

CONDITIONAL MVSS (#3)

7 PERFORMANCE RELATED INPUT VARIABLES ONLY,
5 COST RELATED INPUTS FIXED AT
MODE VALUES

STATISTICS FOR OUTPUT VARIABLE TON

MINIMUM 191.27 MAXIMUM 469.76

MEAN 224.17 VARIANCE 1285.8 STD.DEVIATION 35.858

PERCENTILES: 2.5% 194. 5.0% 196. 50.0% 213. 95.0% 295.

97.5% 315.

Figure 10.1

Conditional MVSS Output Histograms for
Example Photochemical Process

STATISTICS FOR OUTPUT VARIABLE TON

MINIMUM 199.67 MAXIMUM 212.06

MEAN 205.64 VARIANCE 5.0740 STD.DEVIATION 2.2526

PERCENTILES: 2.5% 201. 5.0% 202. 50.0% 206. 95.0% 209. 97.5% 210.

500 POINT HISTOGRAM * = 1 POINTS

PROB	CUME	VALUE			
0.0020	0.0000	199.5		1	*
0.0080	0.0020	200.0		4	****
0.0100	0.0100	200.5	BL	5	*****
0.0120	0.0200	201.0	bin	6	******
0.0140	0.0320	201.5		7	*******
0.0360	0.0460	202.0		18	******************
0.0440	0.0820	202.5		22	**********************
0.0500	0.1260	203.0		25	*************************
0.0680	0.1760	203.5		34	**********************************
0.0720	0.2440	204.0		36	************************************
0.0780	0.3160	204.5		39	***************************************
0.0740	0.3940	205.0		37	************************************
0.1080	0.4680	205.5		54	**
0.0840	0.5760	206.0		42	***
0.0520	0.6600	206.5		26	**************************
0.0880	0.7120	207.0		44	**
0.0580	0.8000	207.5		29	*****************************
0.0360	0.8580	208.0		18	******************
0.0240	0.8940	208.5		12	************
0.0380	0.9180	209.0		19	*******************
0.0120	0.9560	209.5		6	******
0.0120	0.9680	210.0		6	******
0.0120	0.9800	210.5		6	******
0.0060	0.9920	211.0		3	***
0.0000	0.9980	211.5		0	
0.0020	0.9980	212.0		1	*
	1.0000	212.5			

Fig. of Merit TON is Unit Cost of Methanol in $/ton

CONDITIONAL MVSS (#4)

5 COST RELATED INPUT VARIABLES ONLY,
7 PERF. RELATED INPUTS FIXED
AT MODE VALUES.

Figure 10.1 (Continued)

or engineering cost estimates based on inadequate definition of a process.

The final results of the three-way AIS process assessment illustrated this second conclusion nicely. Two of the developers' projected baseline unit costs fell completely below and outside the middle 90% uncertainty range calculated from an MVSS on the respective process models. The winner of the competition, the AVLIS process, had chosen a conservative baseline which fell close to the median of its unit cost uncertainty histogram.

The photochemical process considered in Appendix I also shows a baseline that is optimistic and falls near the 20% point on the uncertainty histogram. This infers that there is a 80% chance that the process will not produce at the projected baseline unit cost. Figure 10.2 (same histogram as Figure 9.9) shows the output histogram and the relative location of the baseline unit cost.

For all of the preceding examples, and as one might expect in light of the first conclusion, most of the misestimation of the proponent's baseline is a result of overestimation of performance. If these developers go back and look at the input variables, $X_i)_{base}$, they used to define their process, they will no doubt find that most of these variables fall on the optimistic sides of their individual input distributions submitted to the Monte Carlo analysis.

The individual developer must weigh carefully the consequences of purposefully making early optimistic baseline projections and then having them possibly discredited when uncertainty analysis is performed. Many institutional and political factors are also involved, hence; there are no

20% by interpolation

$20l/ton BL falls in here

PROB (pdf)	CUME (cdf)	VALUE ($/ton)		FIGURE OF MERIT ION IS $ PER TON OF METHANOL
0.0300	0.0000	190.0	15	***************
0.1320	0.0300	195.0	66	**********
0.1200	0.1620 BL	200.0	60	**********
0.1240	0.2820	205.0	62	**********
0.1000	0.4060	210.0	50	**********
0.0800	0.5060	215.0	40	**********
0.0780	0.5860	220.0	39	**********
0.0480	0.6640	225.0	24	**********
0.0420	0.7120	230.0	21	**********
0.0360	0.7540	235.0	18	**********
0.0340	0.7900	240.0	17	**********
0.0200	0.8240	245.0	10	**********
0.0140	0.8440	250.0	7	*******
0.0200	0.8580	255.0	10	**********
0.0120	0.8780	260.0	6	******
0.0120	0.8900	265.0	6	******
0.0040	0.9020	270.0	2	**
0.0140	0.9060	275.0	7	*******
0.0060	0.9200	280.0	3	***
0.0080	0.9260	285.0	4	****
0.0040	0.9340	290.0	2	**
0.0060	0.9380	295.0	3	***
0.0040	0.9440	300.0	2	**
0.0140	0.9480	305.0	7	*******
0.0000	0.9620	310.0	0	
0.0060	0.9620	315.0	3	***
0.0040	0.9680	320.0	2	**
0.0000	0.9720	325.0	0	
0.0000	0.9720	330.0	0	
0.0020	0.9720	335.0	1	*
0.0040	0.9740	340.0	2	**
0.0040	0.9780	345.0	2	**
0.0000	0.9820	350.0	0	
0.0000	0.9820	355.0	0	
0.0020	0.9820	360.0	1	*
0.0000	0.9840	365.0	0	
0.0000	0.9840	370.0	0	
0.0020	0.9840	375.0	1	*
	0.9860	380.0		

Baseline(BL) would fall in this bin.

STATISTICS FOR OUTPUT VARIABLE TON

MINIMUM 190.69 MAXIMUM 495.19

MEAN 226.89 VARIANCE 1556.1 STD.DEVIATION 39.448

PERCENTILES: 2.5% 194. 5.0% 196. 50.0% 215. 95.0% 306. 97.5% 340.

500 POINT HISTOGRAM * = 1 POINTS

Figure 10.2

Comparison of Example Photochemical Process
Baseline Unit Cost and Unit Cost Histogram

definitive guidelines which can be given to the developer for selecting baseline inputs. It is up to the evaluator to somewhat gauge the degree of development optimism with which he must deal.

An example of developer optimism is the off-cited statement attributed to an early proponent of nuclear power that electricity generated by nuclear fission would be "too cheap to meter." Such optimism is commonplace in development projections, especially for new energy technologies such as solar, fusion, and biomass. Decision makers need a means of discounting unwarranted optimism. Maintaining independence of an economic assessment effort from the R&D organization is one method of improving the objectivity of economic projections.

It should be remembered that credibility of an assessment derives from a demonstration that process performance and system cost projections are validly related to special equipment configurations and conditions of process operation. These relationships constitute the assessment model which was discussed in Chapters V through VII. With proper application of the Monte Carlo technique, the assessment model can be used to provide the decision-maker with credible estimates which bound the likely performance and costs of the project.

Other Observations

The following are other observations and guidelines which are useful to the user of this methodology:

1. The output histogram for unit costs is nearly always positively skewed, i.e., the median unit cost exceeds the mode. This result is due partially to the fact that most input hardware cost distributions are

positively skewed i.e., the analyst believes that more than 50% of the cases submitted for Monte Carlo analysis will involve hardware costs that lie above their distribution mode values. For purely mathematical reasons also, a distribution on a function Y (where Y involves multiplicative relationships between its independent variables X_i), will always be positively skewed.

The low end tail of the unit cost distribution is shorter than the high end tail for two additional reasons also. Even if the process were so good that production could be started at practically no capital expense, one would still encounter operating costs for labor, materials, etc., just for maintaining the support activities common to any process. There is therefore a limiting minimum unit cost against which the low end tail of any unit cost distribution must terminate.

If for some cases submitted to the MVSS the process proves to be nearly infeasible, i.e., it fails to perform anywhere near its projected productivity, the termination of the upper tail of the unit cost distribution can rise to values many times the baseline.

2. This methodology is best utilized for comparison of competing processes at the same or close to the same RD&D level. The level of detail and quality of the models are more likely to be similar.

3. As with all computer calculations, the end results are only as good as the input data and the model itself. As the evaluation effort proceeds, both the input data and the three modules (performance, design, and cost) constituting the overall model should improve significantly in quality.

4. The MVSS method cannot predict the occurrence of breakthroughs or catastrophes in a pioneer process development program or fatal flaws in process theory. Via the use of modeling algorithms it can only translate the effects of changes in key input assumptions to changes in output figures of merit. The technology modeled is assumed to be workable and its productivity capable of calculation from a set of input variables.

5. During the course of an MVSS, it is best to hold global economic indicators, such as the discount rate, inflation rate, deployment schedule, and escalation factors, constant. The discount rate, for example, is just as strong a driver of unit cost as are the technology related cost drivers. Figure 9.6, which includes a sensitivity study for the discount rate utilized in the XYZ assessment model, illustrates this high leverage. For the new processes considered in this methodology, the technology and the associated costs which it drives are the principal issues of interest. A separate uncertainty analysis (task III) utilizing DCF models should be performed on global economic or strategic variables.

6. Considerable care must be taken to ensure that the input variables to the Monte Carlo driver and the model are as nearly independent as possible. Failure to exercise such caution will result in unrealistic or biased cases being generated by the overall model.

7. Global correction factors, such as those described in Chapter VII, should be used only in the earliest models and only to compensate for modeling deficiencies. Other figure-of-merit adjustment factors, such as those proposed in the RAND study on pioneer processes; should only be utilized for processes which fall within the descriptive

data base from which they are derived. Extending them to new and diverse technologies can produce highly misleading and often meaningless results.

Validation

None of the technologies, for which this method of evaluation has been used, has yet reached the large-scale production stage, hence, no data base for actual versus predicted figures of merit exists. Where the method has been extremely successful is in deconvoluting and elucidating the central issues for selection of process technologies such as those for advanced isotope separation. By focusing attention on the important technology-related economic leverage issues, there is less of a tendency for politics and developer salesmanship to predominate a selection decision. It is hoped that other applications for this methodology will appear in the future and well-informed decisions evolve therefrom.

CHAPTER XI

SUGGESTIONS FOR FUTURE RESEARCH

In the preceding sections it was mentioned that lack of historical data on achieved versus predicted costs is a fact of life for many new processes. This is especially true for processes involving first-of-a-kind technologies such as lasers, plasmas, and never-utilized materials. As development and deployment of such technologies proceed, a historical data base begins to accumulate and suggests the basis for possible future studies similar to that of Rand.[88] Only by studying such data can the productive validity of methodology such as that here presented be evaluated and its usefulness and accuracy improved. Obtaining such data will not be an easy task since many developers are loath to divulge information reminding others how incorrect their original predictions were. Such data, however, have the potential of allowing much improved early estimates for subsequent development efforts. Among a particular data base which could be considered is the correlation between the ratio of demonstrated productivity during R&D (in year n) to achieved full-scale productivity (in later year N), and the ratio of achieved full-scale productivity (in year N) to the model predicted full-scale productivity (projection made in year n). These data could be gathered for various classes of technologies.

The application of this methodology to new energy technologies such as fusion and solar electric power generation would by itself be a major and worthwhile undertaking. The MVSS method can perhaps assist in pointing out the particular type of solar or fusion technology which

would benefit most from R&D breakthroughs and at the same time help direct development efforts into those areas which will lead to workable and economic power production processes.

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APPENDICES

APPENDIX A

ACRONYMS

AACE	American Association of Cost Engineers
AGC	Advanced Gas Centrifuge
AIS	Advanced Isotope Separation
AVLIS	Atomic Vapor Laser Isotope Separation
BOP	Balance of Plant
CCG	Capital Cost Growth
cdf	Cumulative Density Function
CRF	Capital Recovery Factor
DCF	Discounted Cash Flow
DTFR	Deviation/Transfer Function/Response
GC	Gas Centrifuge
GCEP	Gas Centrifuge Enrichment Plant
IDC	Interest During Construction
LANL	Los Alamos National Laboratory
LLNL	Lawrence Livermore National Laboratory
LWR	Light Water Reactor
MLIS	Molecular Laser Isotope Separation
MTBF	Mean Time Between Failures
MTTR	Mean Time to Restore
MVSS	Multi-Variable Sensitivity Studies
OCG	Operating Cost Growth
PD	Performance Discount
pdf	Probability Density Function

PDP	Process Delay Penalty
PSP	Plasma Separation Process
RAM	Reliability, Availability, Maintainability
RD&D	Research, Development & Deployment
SVSS	Single Variable Sensitivity Studies
SWU	Separative Work Unit
TEC	Total Estimated Cost
TRW	TRW Incorporated
UCC-ND	Union Carbide Corporation-Nuclear Division
USDOE	United States Department of Energy

APPENDIX B

GLOSSARY OF ECONOMIC ANALYSIS TERMS

The engineering economics and cost estimating literature sometimes use different terminology for what are really the same cost categories. In Peters and Timmerhaus,[89] for example, production costs are broken down into direct costs, fixed charges, overhead, administrative, financing, and distribution and marketing costs. For predictive estimates generated during the early R&D program, the two inclusive categories of capital and operating costs are sufficient for defining annual production costs.

ANNUAL PRODUCTION COSTS: The total levelized costs, both recovered capital and operating, which are associated with the annual production of a predetermined levelized amount of energy or commodity in a large scale facility. Sometimes called TOTAL ANNUALIZED COSTS.

CAPITAL COST: The total capital investment or total estimated cost (TEC) spent for acquisition, installation, and start-up of process and support equipment including construction of a facility to house it. Associated indirect costs such as engineering and contingency should also be included. Most of this money is spent before production begins. If the discounted cash flow method is not used, capital costs can be expressed as a lump sum rather than spread out in a spending pattern over years of construction. In this case the interest during construction covers the cost of the construction loan.

CAPITAL RECOVERY FACTOR (CRF): A multiplier on the lump sum capital costs (including interest during construction) which writes off these costs over a specified period of time and includes a charge for interest on the unrecovered balance, i.e., CRF $= \frac{i}{1-(1+i)^{-n}}$, where i is the interest rate and n is the number of years to write off the capital. This approach is exactly that used to calculate payments on a home mortgage. The product of the lump-sum capital cost and the CRF is added to the annual operating costs in order to form the annualized production costs.

CONVERSION: The conversion of a particular process step represents the fraction of one form of matter or energy converted to another form. The process productivity may depend on several different conversions calculated internal to the productivity and design models. Yields calculated for chemical reactions are related to conversion of the reactants via the stoichiometry.

ONSTREAM EFFICIENCY: This term represents the fraction of time that a process operates at the desired baseline production rate. For many processes this term is synonomous with availability. This term always has a value less than 1.0 and implies that a design must include some extra capacity to compensate for expected downtime or time off stream and still meet the productivity goal.

OPERATING COSTS: Annual costs incurred during routine operation of the plant such as operating labor, replacement materials, utilities, and interest charges on working capital and inventory. If discounted cash

flow is not used, the amortization of the lump sum capital cost over the life of the project, also called capital recovery, is sometimes considered an annual operating cost; however, the latter nomenclature can lead to confusion. The use of the term operating costs here will not include recovered capital. In any case, the total of annual recovered capital and annual operating costs is referred to as the annual production cost or total annualized cost. For purposes of simplification, these costs are expressed on an average annual basis in constant-year dollars and do not vary from year-to-year.

PERFORMANCE: Performance is normally a measure of the extent to which a predetermined and predicted output, or annual productivity, is actually achieved as the process proceeds down the development path. The assessment model is designed to always achieve a nominal performance or constant productivity, P_0, via redesign and reoptimization of the process.

UNIT COST: Dividing the annual production costs, i.e., the total annualized costs, by the calculated annual productivity yields a unit product cost. The unit product cost, which includes the annual operating costs and recovery of the capital costs is usually the figure of merit of most interest at the RD&D Level I-III point in the project life cycle. This figure of merit has the advantage of combining both total annualized costs and performance, i.e., productivity, in a single figure of merit.

APPENDIX C

GLOSSARY OF UNCERTAINTY ANALYSIS TERMS

BIN: A small Δ or range within which a Y value from a given Monte Carlo range can fall. Several bins are required to construct a histogram. For example, an output unit cost of \$0.475/lb might fall in the bin bounded by \$.46/lb and \$.48/lb, i.e., a bin with a Δ of \$.02/lb. A histogram with a range of \$.36 to \$.54/lb would have 9 such bins. In a 500 iteration MVSS, all 500 generated unit costs should be distributed among these 9 bins.

cdf: Cumulative density function. The function, with values ranging from 0 to 1, formed by integration of a pdf, i.e., a probability density function. cdf's are required to generate return values for input variable distributions.

DISTRIBUTION: A general term commonly used to describe a pdf or cdf. The latter two are really mathematical functions described by statistical parameters which model distributions resulting from actual probabilistic events. When a histogram is constructed by the simulation, it represents a distribution.

ENSEMBLE: A single set of uncertainty inputs, X_i, submitted for simulation in a given iteration.

ITERATION: One call of the assessment model (controlled by SUBROUTINE FUNCT) by the Monte Carlo driver code. Represents the submission of one ensemble of inputs.

MEAN: Statistical parameter representing the arithmetic average of all Y_i values (the sample) appearing in a histogram, also the expected value of a pdf.

MEDIAN: Y_i value above which 50% of the total cases in a histogram distribution fall.

MODE: The most likely value (highest probability) in a pdf or distribution.

MVSS: Multi-Variable Sensitivity Study. One ccmplete set of iterations and histograms outputs resulting from a simulation. The key tool for uncertainty analysis.

OUTPUT HISTOGRAM: The distribution of Y_i values resulting from a simulation after placement of the vaues into appropriate bins.

PERCENTILES: The zth percentiles represents the single Y_i value below which z% of the total Y_i values occur.

pdf: Probability density function. The mathematical formulation which represents or models the relative probability of a particular value of a variable X occurring within its range.

RETURN VALUE: The X_i value on the abcissa of a cdf which corresponds to a particular uniformly distributed random number on the ordinate of the same cdf.

SKEWNESS: The location of the mean relative to the mode in a distribution which can be used to describe the shape of the curve.

STANDARD DEVIATION: The statistical parameter which serves as a measure of dispersion of a random variable Y about its mean value.

UNIFORMLY DISTRIBUTED RANDOM NUMBER: A computer generated floating point variable between 0 and 1.0 used to select return values for input cdf's in a simulation.

X-ARRAY: A set of X_j uncertainty inputs constituting an ensemble.

Y-ARRAY: The set of all Y values stored from all iterations in a simulation. The output histogram and statistics are compiled from this array.

APPENDIX D

TALENTS AND RESOURCES REQUIRED FOR A CONTINUING ASSESSMENT EFFORT

Successful application of economic assessment methodology demands that the appropriate forms of material support and organizational effort be applied to a project or system befitting the scope and framework of the proposed evaluation technique.

The first part of this Appendix on required resources is oriented toward two types of managers: the decision-maker, in most cases probably the executive responsible for funding and evaluating R&D programs; and the potential leader of the economic assessment effort, in most instances a person familiar with R&D activities.

The second part of this Appendix is oriented toward the attributes of persons doing the assessment work, referred to as analysts.

Implementation

Success or failure of an economic evaluation effort depends greatly on the success of high-level management in assembling the proper human resources for the task, i.e., the assessment team.

The team leader is the one who must motivate his small staff; understand, but not interfere, with their efforts; and assure that all the pieces of the methodology flow together coherently and in the proper time frame. This person will probably have a team of two to five technical professionals and one or more mathematical or programming assistants. The team leader should be a generalist in his approach to

technical subjects. The team leader must possess a broad overview of the technology, yet understand in adequate detail the major scientific, engineering, and economic issues associated with the process application..

People-oriented skills are also important in the task leader. Much of the information needed for assessment must be obtained from in-house or outside research or development organizations. R&D personnel are often suspicious of those in evaluator roles, hence a low-key amicable approach to acquiring data must be utilized. Allowing R&D personnel to "peer-review" the evaluation methodology and associated models can help promote good working relationships.

Presentation of results is also an important task for the task leader and team. Above average speaking and writing ability are important assets to the team leader, since he will be responsible for briefings and reports to management.

Other Resources

The decision-maker must make other resources available to the assessment team on an as-needed basis. Among the most important are computer facilities and programming specialists, consultants for interpretation of highly specialized areas of scientific and engineering expertise, and cost estimators who can translate design requirements into costs.

The Analysts' Perspective

General Descriptions of Tasks

For purposes of discussion both the team leader and members will be referred to as analysts. Basically two types of staff analysts are

needed: a performance analyst who understands the science issues relating to process design and performance, and an economic analyst who can translate the design and operational consequences associated with performance into costs. Both types will find it necessary to spend considerable time in gathering the data from sources such a RD&D organizations, hardware suppliers, design engineers, cost estimators, and outside consultants. Once initial data are obtained they must be integrated into an entity capable of calculating the needed figures of merit, i.e., a system model. A performance model and an economic model can be developed independently; however, each half of the effort must be aware of the input and output requirements of the other half since ultimately they must be joined. As modeling proceeds and analysis of output data results, the analyst must be able to interpret these to the team leader and prepare the necessary text and visual aids for the reporting of assessment results.

APPENDIX E

A FORTRAN ASSESSMENT MODEL FOR THE REFERENCE XYZ PROCESS

```
      SUBROUTINE FUNCT
C   IN THIS RUN THE BASE CASE WILL OPTIMIZED WITH RESPECT
C     TO FA0 AND XA0 FOR CONSTANT PRODUCTIVITY
C  REACTION EXAMPLE IS FROM LEVENSPIELS'S "CHEM. REACTION ENGRG"
C   FIRST ORDER REACTION (GAS PHASE)
C         A=4R   T=390R,P=3.2 ATM
C   PROCESS VARIABLES:
C         REACTION RATE CONST (EQUIV. TO CATALYST ACTIVITY)
C                K [(LITERS FLUID)/((HR)(LITER CATALYST))]
C   DESIGN VARIABLES:
C        PROCESS FEEDRATE & FEED CONCENTRATION
C                FA    [G-MOLE A/HR]
C                CA0   [G-MOLE A/LITER FLUID]
C   FRACT CHANGE IN VOL UPON REACTION
C                EA    [D'LESS]
C   PLUG FLOW REACTOR VOLUME
C                V     [LITERS OF REACTOR VOL]
C   CONVERSION OF A
C               XA     [DIM;LESS]
C   ECONOMIC VARIABLES
C   COST OF FEED
C                CF0   [$/GM-MOLE A]
C   CAP COST OF REACTOR OF VOLUME V0
C                CR0   [$]
C   CAPITAL RECOVERY FACTOR
C                FCR   [1/YR]
C   CATALYST BULK DENSITY
C                DCAT  [GM CATALYST/LITER OF REACTOR VOL]
C   CATALYST UNIT COST
C                CCAT  [$/GM OF CATALYST]
C   CONSTANT ANNUAL OPERATING COSTS
C                COFIX [$/YR]
C   8760 IS THE NO OF HOURS IN A YEAR
C
C   FIGURES OF MERIT
C   PRODUCTIVITY
C                P   [GM-MOLES R/YR]
C   ANNUAL PRODUCTION COSTS
C                COP   [$/YR]
C   UNIT PRODUCT COST
C                CUNIT  [$/GM-MOLE R]
C***********************************************
```

```
      COMMON/WHY/K,CF0,CCAT,XA0,P0,V,CFEED,CREACT,CCATA,
     *COP,CUNIT,Y(34)
      COMMON/PRINT/ITER,INTER,IPR
      REAL*4 K
C     SET CONSTANTS
C    REFERENCE REACTOR VOLUME
      V0=140.2
C    DESIRED HOURLY PRODUCTION
      P0=2800
C    CONSTANTS
      CA0=0.1
      COMPAR=1.E6
      EA=3.
C    REFERENCE REACTOR CAPITAL COST
      CR0=1.E5
      FCR=.16275
      COFIX=5.E4
      DCAT=5000.
C    PICK VALUE FOR RATE CONSTANT
C    LOOP TO OPTIMIZE CUNIT W/R TO XA0 AND FA0
      DO 100 I=1,100
      XA0=I/100.
      FA0=P0/(4.*XA0)
C    CALC V    (UNOPTIMIZED  VOLUME)
      V=(FA0/(K*CA0))*(((1.+EA)*ALOG(1./(1.-XA0)))-EA*XA0)
C    CALC OF ANNUAL OPERATING COSTS
C     ANNUAL FEED COST
      CFEED=8760.*CF0*FA0
C     REACTOR CAPITAL COST RECOVERY
      CREACT=CR0*((V/V0)**0.6)*FCR
C     CATALYST CAPITAL COST RECOVERY
      CCATA=CCAT*DCAT*V*FCR
C     TOTAL ANNUAL COSTS
      COP=CFEED+CREACT+CCATA+COFIX
C    CALC UNIT COST OF PRODUCT R
      P0AN=P0*8760.
C     CALC UNIT COST OF PRODUCT R
      CUNIT=COP/P0AN
      GO TO 777
C    PRINT OUT RESULTS
      IF(ITER.LE.IPR)
     1WRITE(6,3)I,J
    3 FORMAT('0I    = ',I2,T20,'J    = ',I2)
      IF(ITER.LE.IPR)
     *WRITE(6,1)CA0,FA0,XA0,DCAT,K,V,P0
    1 FORMAT('0CA0 = ',F6.3,T20,'FA0 = ',F6.0,/,
     *' XA0 = ',F6.3,T20,'DCAT = ',F6.0,/,
     *' K    = ',F6.1,T20,'V    = ',F6.1,/,
     *' P0   = ',F6.0,//)
```

```
      IF(ITER.LE.IPR)
     *WRITE(6,2)CFEED,CREACT,CCATA,COFIX,COP,POAN,CUNIT
    2 FORMAT('0CFEED =',T15,F9.0,/,' CREACT =',T15,F9.0,/,' CCATA =',T15
     *,F9.0,/,
     *' COFIX =',T15,F9.0,/,' ',T15,'--------',/,
     *' COP =',T15,F9.0,//,' POAN =  ',F10.0,/,' CUNIT = ',F6.4,//)
  777 CONTINUE

C   COMPARISON OF NEW UNIT COST WITH LAST ONE
      IF(CUNIT.GT.COMPAR) GO TO 111
C   SAVES TH ELAST CASE INCASE IT IS THE MINIMUM CUNIT
      COMPAR=CUNIT
      XX=XA0
      VV=V
      FF=FA0
      CFD=CFEED
      CRT=CREACT
      CC=CCATA
      COPR=COP
      CU=CUNIT
  100 CONTINUE
C  SAVES AND PRINTS THE OPTIMUM CASE
  111 IF(ITER.LE.IPR)WRITE(6,112)
  112 FORMAT(' OPTIMUM CASE',/)
      XA0=XX
      V=VV
      FA0=FF
      CFEED=CFD
      CREACT=CRT
      CCATA=CRT
      COP=COPR
      CUNIT=CU
      IF(ITER.LE.IPR)WRITE(6,1)CA0,FA0,XA0,DCAT,K,V,P0
      IF(ITER.LE.IPR)WRITE(6,2)CFEED,CREACT,CCATA,COFIX,COP,POAN,
     *CUNIT
      RETURN
      END
```

APPENDIX F

A GENERIC FORTRAN CAPITAL COST SCALING MODEL

```
C  WRITING AND FORMATTING STATEMENTS ARE OMITTED
C**********************************************

      SUBROUTINE CAPCOS(Q1,Q1B,Q2,Q2B,Q3,Z,Y,X1,N,C3B,MTTR3,
     *MTBF3,PRATIO,CAPKW,TONS,AREX,PRESS,FLO,VOL,HEAD,
     *HEATLD,POWRI,PWTR,PSTM,POWPB,CSQFT,ATOT,CACRE,FENG,
     *FIDC,FCON)

**************************************************

C COST SCALING EQUATIONS

**************************************************
C FOR PROCESS SPECIFIC ITEMS(TYPICAL EQUATION FORMS)
C THE ACTUAL EQUATIONS ARE TO BE SUPPLIED BY THE ANALYST
****************************************
C COST OF ITEM 1,  WHICH SCALES WITH VARIABLES Q1 &Q2 VIA
C SCALING EXPONENTS( QN1& QN2 ARE THE BASELINE VALUES)
      C1=C1B*(Q1/Q1B)**Z)*(Q2/Q2B)**Y
C COST OF AN ITEM WHICH IS COST SCALABLE VIA AN INPUT
C UNIT ITEM 2 COST VALUE: X2
      C2=X2*Q3
C COST OF 'N' REPLICATED ITEMS 3 OF AVERAGE COST C3B @
      C3=N*C3B
C COST OF SPARES FOR  ITEM 3
      CSPR3=(N*MTTR3/MTBF3)*C3B
C TOTAL SPECIAL PROCESS EQT COST
      CSPEQ=C1+C2+C3+CSPR3
****************************************
C BALANCE OF PLANT ITEMS
C FOR PROCESS AUXILIARIES TYPICAL COST CENTERS AND
C COST DRIVING VARIABLES ARE SHOWN
C THE ACTUAL FUNCTIONS ARE TO BE SUPPLIED BY THE
C ANALYST
C ****************************************
C COMPRESSOR COST (PRATIO=COMPRESSION RATIO)
      CCOMP=F1(PRATIO)
C   GENERATOR COSTS (CAPKW=REQ'D GENERATION CAPACITY)
      CGEN=F2(CAPKW)
C   REFRIGERATION COST (TONS=REQ'D REFRIGERATION CAPACITY)
      CREFR=F3(TONS)
C   HEAT EXCHANGER COST (AREX=REQ'D HEAT TRANSFER TUBE AREA)
      CHEX=F4(AREX)
C   PIPING COST (PRESS=PRESSURE,FLO=FLOWRATE)
      CPIPE=F5(PRESS,FLO)
C   STORAGE TANK COST(PRESS=PRESSURE,VOL=TANK VOLUME)
      CTANK=F6(PRESS,VOL)
```

```
C    PUMP COST (FLO=FLOWRATE,HEAD=VELOCITY HEAD)
       CPUMPS=F7(FLO,HEAD)
C    COOLING WATER SYSTEM AND COOLING TOWERS
C    (HEATLD=TOTAL PLANT HEAT REJECTION LOAD)
       CCW=F8(HEATLD)
C    OUTSIDE UTILITIES INCL. SWITCHGEAR
C    (POWRI=TOTAL PLANT ELECT.LOAD,PWTR=PLANT WATER
C    REQTS,PSTM=PLANT STEAM REQTS)
       COUTS=F9(POWRI,PWTR,PSTM)
C    PROCESS BLDG ELECTRICAL DIST SYSTEM COST
C    (POWPB=PROC.BLDG ELECT. LOAD)
       CEDS=F10(POWPB)
C    PROCESS BUILDING COST (CSQFT=COST PER SQ. FT.OF BLDG AREA,
C    ATOT=TOTAL PROCESS BLDG FLOOR AREA)
       CBLDG=CSQFT*ATOT
C    SITE COST (CACRE=COST PER ACRE FOR RAW LAND)
       CSITE=CACRE*F14(ATOT)
C    THE SCALING OF THESE ITEMS IS PROCESS SPECIFIC:
C    INSTRUMENTATION AND CONTROL
       CIC=F11(Q1,Q2)
C    PRE-OPERATIONAL CHECKOUT &START-UP COST
       CPCHK=F12(Q1,Q2,Q3)
C    SPECIAL SHOPS
       CSS=F13(Q1,Q2)
C    TOTAL COST OF BALANCE OF PLANT ITEMS:
       CBOP=CCOMP+CREFR+CHEX+CPIPE+CTANK+CPUMPS+CCW+COUTS
      *+CEDS+CBLDG+CSITE+CIC+CPCHK+CSS
C    TOTAL DIRECT COST
       CCTOT=CSPEQ+CBOP
C*********************************************
C    CALCULATION OF INDIRECT COSTS(ALLOWANCES)
C*********************************************
C     ENGINEERING (FRACTION FENG SUPPLIED BY COST ESTIMATORS)
       CENG=FENG*CCTOT
C    NEW SUBTOTAL
       C1TOT=CCTOT+CENG
C    CONTINGENCY ANALYSIS(COMPOSITE WEIGHTED CONTINGENCY FRACT,
C    FCON, SUPPLIED BY COST ESTIMATORS)
       CONTT=FCON*C1TOT
C     SUMMATION
       C2TOT=CONTT+C1TOT
C    INTEREST DURING CONSTRUCTION(FIDC CALC FROM CAPITAL SPENDING PATTERN)
       CIDC=FIDC*C2TOT
C*********************************************
C    SUMMATION AND CALC OF TOTAL PLANT CAPITAL
C*********************************************
       CTOTS=(C2TOT+CIDC)
       RETURN
       END
```

APPENDIX G

A GENERIC FORTRAN OPERATING COST SCALING MODEL

```
      CALL OPRCOS(N,MUNIT,MTBF3,MREFB,MAIN1,MAIN3,Q1,Q1B,
     *SFRAC,ADFRAC,F,CFUNIT,C3B,PSPEQ,PCOMP,PPUMP,PIC,PHV,
     *POTHER,ENCAP,ENCAPB,SREQ,CBASEU,ATOT,ATOTB,
     *FDINV,PINV,PUNIT,CTOT,P0,CUNIT)
      STOP
      END
C*********************************************************************
C     SUBROUTINE TO CALCULATE ANNUAL OPERATING COST AND THE
C     UNIT COST OF PRODUCT
C*********************************************************************
      SUBROUTINE OPRCOS(N,MUNIT,MTBF3,MREFB,MAIN1,MAIN3,Q1,Q1B,
     *SFRAC,ADFRAC,F,CFUNIT,C3B,PSPEQ,PCOMP,PPUMP,PIC,PHV,
     *POTHER,ENCAP,ENCAPB,SREQ,CBASEU,ATOT,ATOTB,
     *FDINV,PINV,PUNIT,CTOT,P0,CUNIT)
C*****************************
C     STAFFING COSTS
C*****************************
C    ASSUME 3 SHIFT OPERATION:
      SHIFT=3.
C     CALCULATE THE NUMBER OF WORKERS IN THE 5 MAIN STAFFING CATEGORIES
C    1. OPERATIONS(N=# OF ITEM 3 UNITS IN THE PLANT; MUNIT=# OF WORKERS
C     * NEEDED TO OPERATE EACH UNIT)
      NOPER=N*MUNIT*SHIFT
C    2. REFURBISHMENT STAFFING(N=# OF ITEM 3 UNITS, MTBF3=LIFE OF AN
C       ITEM 3 UNIT; MREFB=#OF STAFF NEEDED TO REFURBISH ONE UNIT)
      NREFB=((8760*N)/(MTBF3))*MREFB*SHIFT
C    3. MAINTENANCE STAFFING(N=SAME AS ABOVE; MAIN3=# OF PERSONS REQD
C       TO MAINTAIN ONE UNIT OF ITEM 3; MAIN1= # OF PERSONS NEEDED
C       TO MAINTAIN ITEM 1; Q1 IS AN ATTRIBUTE WHICH AFFECTS THE AMOUNT
C       OF MAINENANCE REQUIRED FOR ITEM 1)
      NMAIN=N*MAIN3+(Q1/Q1B)*MAIN1
C    4. SUPPORT STAFFING(SFRAC=FRACTION OF TOTAL PROCESS DEDICATED STAFF
C       REQUIRED FOR SUPPORT ACTIVITIES)
      NSUPP=SFRAC*(NOPER+NREFB+NMAIN)
C    5. ADMINISTRATIVE STAFFING(ADFRAC=FRACTION OF DEDICATED PRODUCTION
C       STAFF REQUIRED FOR ADMINISTRATION AND SUPERVISION)
      NADM=ADFRAC*(NOPER+NREFB+NMAIN)
C    TOTAL STAFF COUNT
      NSTAFF=NSUPP+NREFB+NADM+NOPER+NMAIN
C    TOTAL STAFFING COST(AVSAL=AVERAGE SALARY OF PERSON
C    EMPLOYED IN THE PLANT)
      AVSAL=19000.
      SALTOT=NSTAFF*AVSAL
C    FRINGE BENEFITS(FPCT=FRACTION OF BASE SALARY ADDED FOR BENEFITS)
      FPCT=0.35
      FRINGE=SALTOT*FPCT
C    SUBTOTAL
      CSALT1=FRINGE+SALTOT
```

```
C   CONTINGENCY ON STAFFING(CLPCT=FRACTIONAL CONTINGENCY ON STAFFING)
      CLPCT=.2
      CONLAB=CLPCT*CSALT1
C   TOTAL STAFFING COST
      CLABOR=CONLAB+CSALT1
C***********************************
C   REPLACEABLE MATERIALS COSTS
C***********************************
C   FEED COSTS(F=ANNUAL FEEDRATE; CFUNIT=COST PER UNIT OF FEED)
      CFEED=F*CFUNIT
C   REPLACEMENT COSTS(N=# OF ITEM 3 UNIT INSTALLED IN THE PLANT;
C   MTBF3=UNIT 3 LIFETIME; C3B=COST OF A SINGLE UNIT 3;
C   NO LEARNING IS ASSUMED FOR THIS CASE
      NREP3=((N*8760)/MTBF3)
      CREP3=NREP3*C3B
C   OTHER WORK MATERIALS(CSALT1=TOTAL OF ALL BASE SALARIES + FRINGES)
      CAWM=0.07*CSALT1
C   TOTAL REPLACEABLE MATERIALS COSTS
      CMATLL=CREP3+CFEED+CAWM
C   CONTINGENCY ON EXPENDABLES:
      FRCON=.2
      CRCON=FRCON*CMATLL
      CMATL=CMATLL+CRCON
C*****************************
C   UTILITY COSTS
C*****************************
C   ELECTRIC POWER:
C      CALCULATION OF ELECTRIC POWER CONSUMED PER YEAR
C      (PSPEQ=POWER USE BY SPECIAL PROCESS EQUIPMENT,PCOMP=COMPRESSOR
C      POWER USE,PPUMP=PUMP POWER USE, PIC=POWER USE FOR I&C,PHV=
C      POWER USE FOR HEATING &VENTILATION,POTHER=ALL OTHER POWER USE)
      POWER=PSPEQ+PCOMP+PPUMP+PIC+PHV+POTHER
C      COST OF ELECTRIC POWER(CKWHR=POWER RATE IN $/KWHR)
      CKWHR=0.04
      CPOWER=CKWHR*8760*POWER
C   COOLING WATER(ENCAP&ENCAPB=COOLING REQT OF NON-BASE
C   AND BASE PLANTS RESP.)
      CCW=(ENCAP/ENCAPB)*2500.*1.13E4*(30./1.E6)
C   PROCESS STEAM(SREQ=PROCESS STEAM REQT IN 1000S LB/YR;
C   CSTM=STEAM COST IN $/1000 LB DRY STEAM)
      CSTM=2.9
      CSTEAM=SREQ*CSTM
C   OTHER UTILITIES(CBASEU=COST OF OTHER UTIL.IN BASELINE EST;
C   ATOT&ATOTB=NON-BASE AND BASE PROCESS BLDG FLOOR AREAS)
      COTHL=CBASEU*(ATOT/ATOTB)
C   TOTAL UTILITIES
      CUTIL=CPOWER+CSTEAM+CCW+COTHL
C************************************
C   INTEREST ON WORKING CAPITAL
C************************************
      CIOWC=0.1*(2./12.)*(CLABOR+CMATL+CUTIL)
```

```
C*********************************
C     INTEREST ON INVENTORIES
C*********************************
C    CALC. VALUE OF FEED AND PRODUCT IN INVENTORY
C    (FDINV,PINV=INVENTORIES OF FEED&PRODUCT; CFUNIT&PUNIT ARE
C    EST. UNIT COSTS)
       CINV=FDINV*CFUNIT+PINV*PUNIT
C    APPLY INTEREST RATE:
       RINT=0.1
       CIOI=RINT*CINV
C    SUBTOTAL
C*********************************
C    TOTAL YEARLY OPERATING COSTS
C*********************************
       CANlT=(CLABOR+CMATL+CIOI+CUTIL+CIOWC)
C*********************************
C    AMORTIZATION
C*********************************
C    CALC OF CAPITAL RECOVERY FACTOR
C       (RINT=INTEREST RATE,NCAMP=# OF YEARS OVER WHICH PLANT IS
C      WRITTEN OFF
       NCAMP=25
       CAPREC=RINT/(1.-(1.+RINT)**(-NCAMP))
       CAPCOS=CTOT
       CAMORT=CAPREC*CAPCOS
C    TOTAL ANNUAL COSTS
       ANCOST=CAMORT+CANlT
C*************************************
C    CALCULATION OF UNIT COST
C*************************************
       CUNIT=ANCOST/(P0)
C     TOTALS
       WRITE(6,706)
  706 FORMAT(10X,'* * * TOTAL ANNUAL OPERATING COSTS IN THOUSANDS OF
     1DOLLARS * * *',//)
       WRITE(6,707)NSTAFF,SALTOT,FPCT,FRINGE,CSALTl,CLPCT,CONLAB,
     1CLABOR,F,CFUNIT,CFEED,NREP3,C3B,CREP3,CAWM,CMATLL,CRCON,CMATL,
     2POWER,CKWHR,CPOWER,CSTEAM,CCW,COTHL,CUTIL,CIOWC,CIOI,
     3CANlT,CTOT,CAPREC,CAMORT,RINT,NCAMP,ANCOST
       RETURN
       END
```

APPENDIX H

A FORTRAN ASSESSMENT MODEL FOR THE XYZ PROCESS
INCLUDING COST SCALING ALGORITHMS

```
C**************************************
C   THIS IS THE OVERALL PROCESS MODEL
C   CALLED BY THE MONTE CARLO DRIVER CODE
C******************************************
      SUBROUTINE FUNCT
C   IN THIS RUN THE BASE CASE WILL OPTIMIZED WITH RESPECT
C     TO FA0 AND XA0 FOR CONSTANT PRODUCTIVITY
C  REACTION EXAMPLE IS FROM LEVENSPIELS'S "CHEM. REACTION ENGRG"
C   FIRST ORDER REACTION (GAS PHASE)
C         A=4R   T=390R,P=3.2 ATM
C   PROCESS VARIABLES:
C         REACTION RATE CONST (EQUIV. TO CATALYST ACTIVITY)
C                K [(LITERS FLUID)/((HR)(LITER CATALYST))]
C   DESIGN VARIABLES:
C        PROCESS FEEDRATE & FEED CONCENTRATION
C                 FA    [G-MOLE A/HR]
C                 CA0   [G-MOLE A/LITER FLUID]
C   FRACT CHANGE IN VOL UPON REACTION
C                 EA    [D'LESS]
C   PLUG FLOW REACTOR VOLUME
C                 V     [LITERS OF REACTOR VOL]
C   CONVERSION OF A
C                XA     [DIM;LESS]
C   ECONOMIC VARIABLES
C   COST OF FEED
C                 CF0   [$/GM-MOLE A]
C   CAP COST OF REACTOR OF VOLUME V0
C                 CR0   [$]
C   CAPITAL RECOVERY FACTOR
C                 FCR   [1/YR]
C   CATALYST BULK DENSITY
C                 DCAT  [GM CATALYST/LITER OF REACTOR VOL]
C   CATALYST UNIT COST
C                 CCAT  [$/GM OF CATALYST]
C
C   FIGURES OF MERIT
C   PRODUCTIVITY
C                 P   [GM-MOLES R/YR]
C   ANNUAL PRODUCTION COSTS
C                 COP  [$/YR]
C   UNIT PRODUCT COST
C                 CUNIT  [$/GM-MOLE R]
C**********************************************
      COMMON/WHY/K,CF0,CCAT,XA0,P0,V,CTOTS,
     *COP,CUNIT,Y(36)
      COMMON/PRINT/ITER,INTER,IPR
      COMMON/WRITE/IOPT
      REAL*4 K
C     SET CONSTANTS
```

```
C   DESIRED HOURLY PRODUCTION
      P0=2800.
C   CONSTANTS
C    FEED CONCENTRATION
      CA0=0.1
C   OPTIMIZER RESET
      COMPAR=1.E6
C   OPTIMIZER PRINT RESET
      IOPT=0
C   VOL CHANGE DUE TO STOICHIOMETRY
      EA=3.
C   CATALYST DENSITY
      DCAT=5000.
C    VALUE FOR RATE CONSTANT IS AN INPUT
C   PRINT OUT INPUTS
      IF(ITER.LE.IPR) WRITE(6,1117)ITER
 1117 FORMAT(1H1,'***OPTIMIZATION OF ',I4,'TH ITERATION***',//)
      IF(ITER.LE.IPR)
     *WRITE(6,1)CA0,DCAT,K,P0
    1 FORMAT('0CA0 = ',F6.3,/,
     *' DCAT = ',F6.0,/,
     *' K    = ',F6.1,/,
     *' P0   = ',F6.0,//)
C   LOOP TO OPTIMIZE CUNIT W/R TO XA0 AND FA0
      DO 100 I=1,100
      XA0=I/100.
      FA0=P0/(4.*XA0)
C   CALC V    (UNOPTIMIZED  VOLUME)
      V=(FA0/(K*CA0))*(((1.+EA)*ALOG(1./(1.-XA0)))-EA*XA0)
C   CALL THE CAPITAL COST SUBROUTINE
C***********************************
      CALL CAPCOS(FA0)
C***********************************
C
C   CALL THE OPERATING COST SUBROUTINE
C***********************************
      CALL OPRCOS(FA0)
C****************************************
C   PRINT OUT THE UNIT COSTS FROM OPTIMIZER ITERATIONS:
      IF(ITER.LE.IPR) WRITE(6,333)I,XA0,FA0,V,CUNIT
  333 FORMAT(' I    = ',I2,T12,'XA0 = ',F6.2,T27,'FA0 = ',F8.1,
     *T47,'V = ',F6.1,T62,'CUNIT = ',F7.4,/)

C   COMPARISON OF NEW UNIT COST WITH LAST ONE
      IF(CUNIT.GT.COMPAR) GO TO 111
C   SAVES TH ELAST CASE INCASE IT IS THE MINIMUM CUNIT
      COMPAR=CUNIT
      II=I
      XX=XA0
      VV=V
```

```
      FF=FA0
      CU=CUNIT
  100 CONTINUE
C  SAVES AND PRINTS THE OPTIMUM CASE
C  PRINT OUT MVSS VARIABLES
  111 IF(ITER.LE.IPR)WRITE(6,1113)ITER
 1113 FORMAT(1H1,'********* MVSS VARIABLE INPUTS AND OUTPUTS FOR '
     *,I4,'TH ITERATION***********
     *****',//)
      IF(ITER.LE.IPR)WRITE(6,1112)ITER,IPR,K,CF0,CCAT
 1112 FORMAT(' ITER = ',I4,'  IPR = ',I2,'  K = ',F6.0,'  CF0 = ',F6.3,
     *'  CCAT = ',F7.2,/)
      IF(ITER.LE.IPR)WRITE(6,112)
  112 FORMAT(' OPTIMUM CASE',/)
      IOPT=1
      I=II
      XA0=XX
      V=VV
      FA0=FF
      IF(ITER.LE.IPR)WRITE(6,1)CA0,DCAT,K,P0
      IF(ITER.LE.IPR)WRITE(6,333)I,XA0,FA0,V,CUNIT
      CALL CAPCOS(FA0)
      CALL OPRCOS(FA0)
      RETURN
      END
C
C
C*********************************************

      SUBROUTINE CAPCOS(FA0)

      COMMON/WHY/K,CF0,CCAT,XA0,P0,V,CTOTS,
     *COP,CUNIT,Y(36)
      COMMON/PRINT/ITER,INTER,IPR
      COMMON/WRITE/IOPT
************************************************
C   CONSTANTS(FROM COST ESTIMATE PERFORMED ON PREVIOUS OPTIMIZED
C   REFERENCE CASE)
C    ENGINEERING ALLOWANCE
      FENG=0.3
C    CONTINGENCY ALLOWANCE
      FCON=0.32
C    INTEREST DURING CONSTRUCTION ALLOWANCE
      FIDC=0.18
C    REACTOR VOLUME(LITERS) IN REFERENCE OPT. DES
      V0=283.
C    ESTIMATED REACTOR COST($) FOR V0 ABOVE
      CR0=1.5E5
C    CATALYST DENSITY(G/LITER)
      DCAT=5000.
```

```
C     CONVERSION IN OPTIMIZED REFERENCE DESIGN
      XA00=0.70
C     FEEDRATE(GMOL A/HR) IN OPTIMIZED REF DESIGN
      FA00=1000.

C COST SCALING EQUATIONS

*************************************************
C  PROCESS SPECIFIC ITEMS
*************************************
C COST OF REACTOR,  WHICH SCALES WITH VARIABLE V  VIA
C SCALING EXPONENTS( V0 IS THE BASELINE VALUE)
      C1=CR0*((V/V0)**0.6)
C COST OF CATALYST WHICH IS COST SCALABLE VIA AN INPUT
C UNIT ITEM  COST VALUE: CCAT
      C2=CCAT*DCAT*V
C   COST OF THE SEPARATOR FOR COMPOUINDS A & R
      C3=3.E4*(XA00/XA0)**0.7
C TOTAL SPECIAL PROCESS EQT COST
      CSPEQ=C1+C2+C3
*************************************
C BALANCE OF PLANT ITEMS
C *************************************
C COMPRESSOR COST
      CCOMP=15.E3*(FA0/FA00)
C   HEAT EXCHANGER COST (AREX=REQ'D HEAT TRANSFER TUBE AREA)
      AREX=XA0*100.
      CHEX=70.*AREX**0.83
C   PIPING COST
      CPIPE=6.E3*(FA0/FA00)
C   STORAGE TANK
      CTANK=20.E3*(FA0/FA00)**.6
C   OUTSIDE UTILITIES INCL. SWITCHGEAR
      COUTS=9.E4
C   PROCESS BLDG ELECTRICAL DIST SYSTEM COST
      CEDS=7.E4
C   PROCESS BUILDING COST (CSQFT=COST PER SQ. FT.OF BLDG AREA,
C   ATOT=TOTAL PROCESS BLDG FLOOR AREA)
      ATOT=4.E3*(V/V0)
      CSQFT=130.
      CBLDG=CSQFT*ATOT
C   SITE COST (CACRE=COST PER ACRE FOR RAW LAND)
      ACRE=((SQRT(ATOT)+150.)**2)/43560.
      CSITE=10.E3*ACRE
C   INSTRUMENTATION AND CONTROL
      CIC=1.E4
C   PRE-OPERATIONAL CHECKOUT &START-UP COST
      CPCHK=5.E4
```

```
C   TOTAL COST OF BALANCE OF PLANT ITEMS:
      CBOP=CCOMP+CHEX+CPIPE+CTANK+COUTS
     *+CEDS+CBLDG+CSITE+CIC+CPCHK
C   TOTAL DIRECT COST
      CCTOT=CSPEQ+CBOP
C*********************************************
C   CALCULATION OF INDIRECT COSTS(ALLOWANCES)
C*********************************************
C    ENGINEERING (FRACTION FENG SUPPLIED BY COST ESTIMATORS)
      CENG=FENG*CCTOT
C   NEW SUBTOTAL
      C1TOT=CCTOT+CENG
C   CONTINGENCY ANALYSIS(COMPOSITE WEIGHTED CONTINGENCY FRACT,
C   FCON, SUPPLIED BY COST ESTIMATORS)
      CONTT=FCON*C1TOT
C    SUMMATION
      C2TOT=CONTT+C1TOT
C   INTEREST DURING CONSTRUCTION(FIDC CALC FROM CAPITAL SPENDING PATTERN)
      CIDC=FIDC*C2TOT
C*********************************************
C   SUMMATION AND CALC OF TOTAL PLANT CAPITAL
C*********************************************
      CTOTS=(C2TOT+CIDC)
C     PRINT OUT
      IF(IOPT.NE.1) GO TO 777
      IF(ITER.LE.IPR)
     *WRITE(6,405)
  405 FORMAT(1H1,
     *T10,'* * * PLANT CAPITAL COST ESTIMATE * * THOUSANDS OF $',
     *//)
      IF(ITER.LE.IPR)
     *WRITE(6,401)C1,C2,C3,CSPEQ
  401 FORMAT(10X,'SPECIAL EQUIPMENT ITEM 1(REACTOR)
     *',T52,-3PF12.1,/,
     *10X,'SPECIAL EQUIPMENT ITEM 2(CATALYST)
     *',T52,-3PF12.1,/,
     *10X,'SPECIAL EQPT ITEM 3(SEPARATOR)',T52,-3PF12.1,/,
     *10X,T52,'------------',/,
     *10X,'TOTAL SPECIAL EQUIPMENT COST',T52,-3PF12.1,/)
      IF(ITER.LE.IPR)
     *WRITE(6,403)CCOMP,CHEX,CPIPE,CTANK,COUTS,
     *CEDS,CIC,CPCHK,CBLDG,CSITE,CBOP
  403 FORMAT(10X,'COMPRESSOR',T52,-3PF12.1,/
     *10X,'HEAT EXCHRS',T52,-3PF12.1,/,
     *10X,'PIPING',T52,-3PF12.1,/,
     *10X,'STORAGE TANK',T52,-3PF12.1,/,
     *10X,'OUTSIDE UTILITIES(INCL. SWITCHGEAR)',T52,-3PF12.1,/,
     *10X,'ELECTRICAL DISTRIBUTION SYSTEM',T52,-3PF12.1,/,
     *10X,'INSTRUMENTATION AND CONTROL',T52,-3PF12.1,/,
```

```
     *10X,'PRE-OPERATIONAL CHECKOUT& STARTUP',T52,-3PF12.1,/,
     *10X,'BUILDING',T52,-3PF12.1,/,
     *10X,'SITE',T52,-3PF12.1,/,
     *10X,T52,'------------',/,
     *10X,'BOP SUBTOTAL',T52,-3PF12.1,//)
      IF(ITER.LE.IPR)
     *WRITE(6,402)CCTOT
  402 FORMAT('0',T52,'------------',/,10X,'TOTAL DIRECT COSTS',
     *T52,-3PF12.1,/,' ',T52,'------------',/)
      IF(ITER.LE.IPR)
     *WRITE(6,406)FENG,CENG,C1TOT,FCON,CONTT,C2TOT,FIDC,CIDC,
     1CTOTS
  406 FORMAT(10X,'ENGINEERING AT ',2PF6.3,' % OF DIRECT COSTS',T52,
     *-3PF12.1,/,T52,'------------',/,10X,'SUBTOTAL',T52,-3PF12.1,/,
     *10X,'CONTINGENCY AT ',2PF6.3,' % OF ABOVE',T52,-3PF12.1,/,
     *T52,'------------',/,10X,'SUBTOTAL',T52,-3PF12.1,/,
     *10X,'INTEREST DURING CONSTRUCTION AT ',2PF6.3,' %',T52,-3PF12.1,
     */,T52,'------------',/,10X,'TOTAL CAPITAL COST',T52,-3PF12.1,//)
  777 CONTINUE
      RETURN
      END
C*************************************************************************
C    SUBROUTINE TO CALCULATE ANNUAL OPERATING COST AND THE
C    UNIT COST OF PRODUCT
C*************************************************************************
      SUBROUTINE OPRCOS(FA0)
      COMMON/WHY/K,CF0,CCAT,XA0,P0,V,CTOTS,
     *COP,CUNIT,Y(36)
      COMMON/PRINT/ITER,INTER,IPR
      COMMON/WRITE/IOPT
C*****************************
C   CONSTANTS
C    REF FEEDRATE
      FA00=1000.
C    REFERENCE ANNUAL PRODUCTIVITY
      P0AN=8760.*2800.
C    REFERENCE POWER CONSUMPTION(KW)
      POW00=440.
C    STAFFING COSTS
C*****************************
C   ASSUME 3 SHIFT OPERATION:
      SHIFT=3.
C   OPERATIONS
      NOPER=2*(FA0/FA00)*SHIFT
C   MAINTENANCE STAFFING
      NMAIN=3*(FA0/FA00)*SHIFT
C   SUPPORT STAFFING(SFRAC=FRACTION OF TOTAL PROCESS DEDICATED STAFF
C      REQUIRED FOR SUPPORT ACTIVITIES)
      NSUPP=SFRAC*(NOPER+NREFB+NMAIN)
```

```
C   ADMINISTRATIVE STAFFING
      NADM=3
C   TOTAL STAFF COUNT
      NSTAFF=NSUPP+NADM+NOPER+NMAIN
C   TOTAL STAFFING COST(AVSAL=AVERAGE SALARY OF PERSON
C   EMPLOYED IN THE PLANT)
      AVSAL=19000.
      SALTOT=NSTAFF*AVSAL
C   FRINGE BENEFITS(FPCT=FRACTION OF BASE SALARY ADDED FOR BENEFITS)
      FPCT=0.35
      FRINGE=SALTOT*FPCT
C   SUBTOTAL
      CSALT1=FRINGE+SALTOT
C   CONTINGENCY ON STAFFING(CLPCT=FRACTIONAL CONTINGENCY ON STAFFING)
      CLPCT=.2
      CONLAB=CLPCT*CSALT1
C   TOTAL STAFFING COST
      CLABOR=CONLAB+CSALT1
C************************************
C   REPLACEABLE MATERIALS COSTS
C************************************
C   FEED COSTS(F=ANNUAL FEEDRATE; CFUNIT=COST PER UNIT OF FEED)
      F=8760.*FA0
      CFEED=F*CF0
C   OTHER WORK MATERIALS(CSALT1=TOTAL OF ALL BASE SALARIES + FRINGES)
      CAWM=0.07*CSALT1
C   TOTAL REPLACEABLE MATERIALS COSTS
      CMATLL=CFEED+CAWM
C   CONTINGENCY ON EXPENDABLES:
      FRCON=.2
      CRCON=FRCON*CMATLL
      CMATL=CMATLL+CRCON
C*****************************
C   UTILITY COSTS
C*****************************
C   ELECTRIC POWER:
      POWER=POW00*(FA0/FA00)
C      COST OF ELECTRIC POWER(CKWHR=POWER RATE IN $/KWHR)
      CKWHR=0.04
      CPOWER=CKWHR*8760*POWER
C   OTHER UTILITIES
      COTHL=40.E3
C   TOTAL UTILITIES
      CUTIL=CPOWER+COTHL
C************************************
C   INTEREST ON WORKING CAPITAL
C************************************
      CIOWC=0.1*(2./12.)*(CLABOR+CMATL+CUTIL)
```

```
C*******************************
C    INTEREST ON INVENTORIES
C*******************************
C   CALC. VALUE OF FEED AND PRODUCT IN INVENTORY
      CPEST=.08
      CINV=100000.*CF0+10000.*CPEST
C   APPLY INTEREST RATE TO CINV:
      RINT=0.1
      CIOI=RINT*CINV
C   SUBTOTAL
C*********************************
C   TOTAL YEARLY OPERATING COSTS
C*********************************
      CANLT=(CLABOR+CMATL+CIOI+CUTIL+CIOWC)
      COP=CANLT
C*******************************
C   AMORTIZATION
C*********************************
C   CALC OF CAPITAL RECOVERY FACTOR
C      (RINT=INTEREST RATE,NCAMP=# OF YEARS OVER WHICH PLANT IS
C     WRITTEN OFF
      NCAMP=10
      CAPREC=RINT/(1.-(1.+RINT)**(-NCAMP))
      CAPCOS=CTOTS
      CAMORT=CAPREC*CAPCOS
C   TOTAL ANNUAL COSTS
      ANCOST=CAMORT+CANLT
C************************************
C   CALCULATION OF UNIT COST
C************************************
      CUNIT=ANCOST/(P0AN)
C    TOTALS
      IF(IOPT.NE.1) GO TO 778
      IF(ITER.LE.IPR)
     *WRITE(6,706)
  706 FORMAT(1H1,
     *10X,'* * * TOTAL ANNUAL OPERATING COSTS IN THOUSANDS OF
     1DOLLARS * * *',//)
      IF(ITER.LE.IPR)
     *WRITE(6,707)NSTAFF,SALTOT,FPCT,FRINGE,CSALT1,CLPCT,CONLAB,
     1CLABOR,F,CF0,CFEED,CAWM,CMATLL,CRCON,CMATL,
     2POWER,CKWHR,CPOWER,COTHL,CUTIL,CIOWC,CIOI,
     3CANLT,CTOTS,CAPREC,CAMORT,RINT,NCAMP,ANCOST
  707 FORMAT(10X,'LABOR COSTS:',/,13X,'TOTAL DIRECT LABOR COSTS FOR
     1 A STAFF OF ',I3,T60,-3PF9.1,/,13X,'FRINGE BENEFITS AT ',2PF5.1,
     2' %',T60,-3PF9.1,/,T60,'---------',/,13X,'SUBTOTAL',T60,-3PF9.1,/,
     313X,'CONTINGENCY AT ',2PF5.1,' %',T60,-3PF9.1,/,T60,'---------
     4---------',/,13X,'TOTAL LABOR COSTS:',T70,-3PF9.1,//,
```

```
     510X,'REPLACEMENT & MATERIAL COSTS:',/,13X,0PE6.1,' UNITS O
     6F FEED @ $ '0PF6.3,' @ ',T60,-3PF9.1,/,
     8/,13X,'ADDITIONAL WORK MATLS
     9',T60,-3PF9.1,/,T60,'----------',/,13X,
     *'TOTAL REPLAC.& MATERIALS COSTS',T70,-3PF9.1,/,
     *13X,'CONTINGENCY AT 20%',T60,-3PF9.1,/,T60,'----------',/
     *13X,'TOTAL EXPENDABLES COST:',T70,-3PF9.1,
     *//,10X,'UTILITY CO
     *STS:',/,13X,0PF6.0,'KW ELECTRIC POWER AT ',0PF5.2,
     *' PER KW-HR',T60,
     *-3PF9.1,/
     *,13X,'OTHER  UTILITIES',T60,
     *-3PF9.1,/,T60,'----------',/,T14,'TOTAL UTILITY COST',
     *T70,-3PF9.1,//,10X,'INTEREST ON WORKING CAPITAL',T70,-3PF9.1,/
     *10X,'INTEREST ON INVENTORIES',T70,-3PF9.1,
     */,T70,'----------',/,10X,'SUBTOTAL ANNUAL COSTS',T69,-3PF10.1,//,
     *10X,'AMORTIZATION OF CAPITAL',/,10X,'($',0PF12.0,' AT CAPITAL
     * RECOVERY OF ',0PF7.4,')',T70,-3PF9.1,/,' ',T26,'I.E. '
     *,2PF5.1,'% INTEREST OVER ',I2,' YRS:',/,T70,'----------',/,
     *10X,'TOTAL ANNUAL COSTS',T70,-3PF9.1,///)
      IF(ITER.LE.IPR)
     *WRITE(6,4)POAN,CUNIT
   4 FORMAT(' UNIT COST FOR PRODUCTIVITY OF',0PE8.2,' UNITS/YR
     *:',T50,F7.3,/)
 778 CONTINUE
     RETURN
     END
```

APPENDIX I

A CONCEPTUAL, FIRST-OF-A-KIND EXAMPLE PROCESS FOR ECONOMIC ANALYSIS: PHOTOCHEMICAL REMOVAL OF SULFUR FROM SYNTHETIC FUELS FEEDSTOCKS

Preface

This evaluation methodology is best understood in the framework of a particular example technology. Although originally developed for use in the evaluation of advanced technologies for uranium isotope separation, the general principles of this methodology are, of course, applicable to a wide variety of process technologies. For example, given a reasonable foundation in the physics and engineering of fusion energy, one could apply the same economic assessment methodology to fusion technologies.

Because of the national security implications of uranium enrichment technology it was decided to demonstrate the methodology on a different proposed high risk energy related application. The example chosen is a different application of the science of laser photochemistry.[90] Before considering process and modeling details, it is beneficial to provide some background information on this generic technology and a few of its elementary principles. A report[91] prepared in 1978 for the U.S. Department of Energy contained much of this background information on photochemistry and the highlights from it are summarized in this next subsection.

Photochemistry: Background Concepts

Scientific Bases

In photochemical processes electromagnetic radiation, usually in the

form of high intensity infrared, visible, or ultraviolet light generated by lasers, is used to supply the necessary activation energy to initiate a chemical reaction. By tuning the laser to resonance with an electronic or vibrational transition in one species in a mixture, a selective reaction of that species alone can be made to occur. Resonant excitation of the desired species (e.g., an isotope, isomer, or impurity) is obtained by irradiation with the very narrow bandwidth light generated by the laser. This bandwidth must be smaller than the difference in the spectroscopic absorption frequencies of the two isotopic or chemical species to be separated. For isotope separation the frequency difference ($\Delta\nu$) is known as the isotopic shift.

In general the equation for a photochemical reaction is

$$A + h\nu \rightarrow A^* \qquad \text{(excitation)}$$

$$AB + h\nu \rightarrow A + B \qquad \text{(dissociation)} .$$

where:

h = Planck's constant (6.63×10^{-34} joule-sec) and

ν = radiation frequency (Hz).

The total quantum energy, $h\nu$, of the photon (or multiple photons) must contain the same amount of energy as the activation energy of the desired reaction (on a per-atom or per-molecule basis). One advantage of lasers in chemistry lies in their monochromaticity or narrow wavelength band which allows for particular reactions to be driven selectively. Another advantage is their high intensity, which means many photons per molecule or atom can be delivered in very short periods, i.e., even nanoseconds, in order to enhance a reaction.

Photochemistry may prove useful for reactions in which trace amounts of a particular component are present and need to be removed. Conventional chemical separation methods for removal of trace quantities can prove futile due to the fact that chemical equilibrium and the thermodynamics of mixtures never allow a complete separation to be effected. Because of high selectivity and high reaction rate, however, laser chemistry exhibits nonequilibrium behavior and allows almost complete excitation of one particular species without affecting other constituents. This behavior is most prevalent in the vapor phase where the collisional and electronic phenomena associated with condensed phases are less likely to redistribute the selectively absorbed energy among neighboring species and destroy any chance of separation.

General Comments on Applications

In the spring of 1978 the U.S. Department of Energy asked a scientific committee (JASON) to conduct a short term study[91] into the potential of laser induced photochemistry for near-term applications in industry, but not to include the production of fissionable isotopes or the goals of basic photochemistry research.

The specific areas of inquiry addressed by the study were near term applications, limitations, energy efficiency, and possible U.S. DOE support. The study made use of many illustrative comparisons between conventional and laser photochemistry, some of which are discussed here.

Conventional photochemistry, in which non-laser light sources are used, is an academic field with an extensive literature extending back over many decades. There are several important industrial processes which involve a photochemical step, for example, the synthesis of

nylon-6 or the synthesis of vitamin D_3. However, industrial photochemical processes are surprisingly scarce when one considers the scientific maturity of the field. Many large chemical firms have made periodic studies of the potential of conventional photochemistry[92] and the conclusions of these studies have been that, with a few exceptions, thermal and pressure control of chemical processes and the use of conventional catalysts is more economical than photochemical processes.

Conventional photochemical processes[93] make use of relatively weak light from sources such as mercury discharge lamps or high pressure xenon or mercury arcs. The ultraviolet lines of the mercury lamp are especially useful, since a large number of photochemical processes with hydrocarbons require ultraviolet light for initiation. Some photochemical processes can also be initiated with visible light, but almost no conventional photochemistry is done with infrared wavelengths ($10^{-4} < \lambda < 10^{-1}$ cm) since very few chemical bonds are weak enough to be broken by the energy of a single infrared photon. Furthermore, at total gas pressures of only a few torr, relaxation of vibrational and rotational energy to translational energy occurs so rapidly that conventional infrared light sources simply cause slight heating of the reagents.

Laser light sources have drastically changed many aspects of photochemistry. Some of the unique properties of laser light as a source of photons for photochemical processes are the following:

1. The high intensity and the spatial and temporal coherence of laser light (implying that the light waves in the laser beam are in phase) make possible nonlinear excitation of chemical species; i.e.,

coherent, intense light has not only the ability to excite molecules, but also the ability to alter their inherent vibrational spectra. A good example is multiphoton excitation and dissociation of molecules such as SF_6 with infrared lasers. Multiphoton excitation in the infrared has made infrared photochemistry possible for the first time. The ultimate utility of infrared photochemistry, however, is not yet established.

2. Laser light sources are now available over large regions of the spectrum from the infrared to the ultraviolet. For conventional photochemistry it is necessary to rely either on quasi-continuous light from arc lamps or on a few intense lines which are available from atomic vapor lamps, such as mercury vapor, to obtain large amounts of nearly monochromatic light.

3. Short pulses of intense laser light are available. Short intense pulses can be used to ensure that monomolecular chemical reactions can be driven to completion before deleterious collisional effects occur; such times are often on the order of microseconds or less.

4. Highly collimated laser light can be focused into reaction chambers through small optical windows. In contrast, conventional lamps emit such diffuse light that the lamp must either be immersed in the reagent or very large transparent windows must be supplied to ensure efficient transfer of light from the lamp into the reaction chamber. Fouling of the large surface areas of transparent windows and lamps is one of the most troublesome practical problems in conventional industrial photochemical processes. Thus, the high spatial coherence of laser light could be a telling advantage in industrial applications,

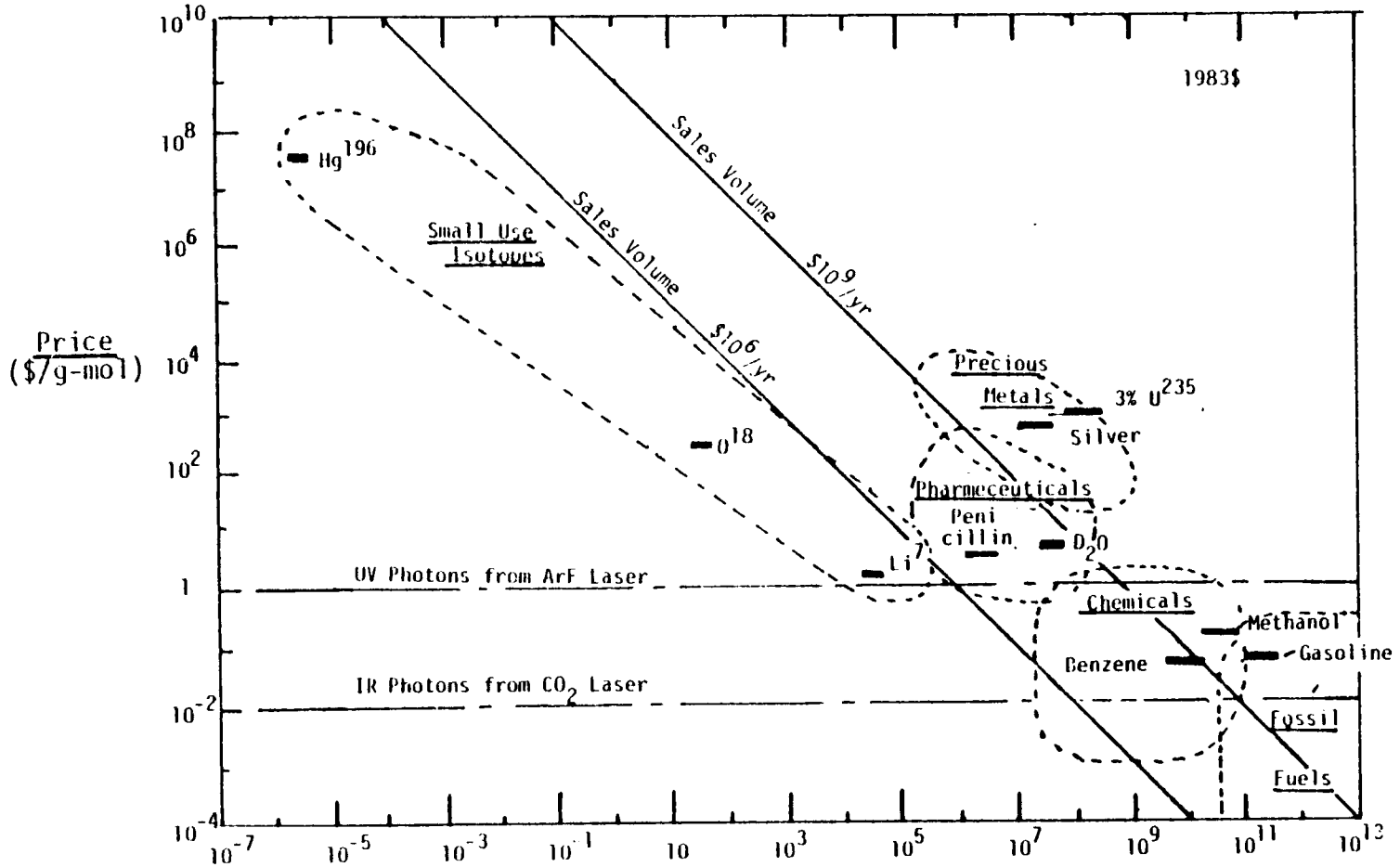
since window fouling problems could be greatly reduced, for example, by the use of small aerodynamically protected windows.

5. Another important practical advantage of highly collimated laser light is the possibility of multiple reflections of the laser beam through weakly absorbing substances. Diffuse conventional light sources are of little use when the attenuation length of the material is very long, since only a small fraction of the available photons is absorbed. Incoherent light from diffuse sources is also more difficult to propagate uniformly through even such weakly absorbing media.

The preceding list of properties from the JASON report[94] is not meant to be exhaustive, but it does show that there are profound differences between lasers and conventional light sources. One might therefore hope that these novel features of laser light could change the economics of industrial photochemistry.

Economic Considerations

The unit production cost for industrial chemicals is often difficult to determine because of proprietary secrecy. However, prices are well known, and any proposed use of laser photochemistry should definitely not add more to the cost of production of a chemical than the anticipated selling price. Some interesting data on chemical prices are shown in Fig. I.1. Note that most high-volume chemicals and fuels sell in the range \$0.01 to \$1 per pound or \$0.001 to \$1.0/g-mol. The costs of feedstocks for such chemicals are small but not negligible. For example, crude oil at \$30 per barrel costs about \$0.125 per pound; coal at \$30 per ton costs \$0.015 per pound. Some molecular weights for common industrial chemicals are: methane, 16 grams/gram mole or 28 gram



Source: Happer,W. et al, (JASON committee), "Laser Induced Photochemistry," SRI International (JSR-78-11) Feb.1979

Figure I.1

A Chemical Price-Annual Production Correlation with Laser Photon Costs Superimposed

moles per pound; benzene, 78 grams/gram mole or 5.8 gram moles per pound; aspirin, 180 grams/gram mole or 2.5 gram moles per pound. Thus the price per gram mole of most industrial compounds is also usually less than $1.0.

As can be seen in Fig. I.1, the production cost of separated isotopes is very high and much of the cost is associated with the thermodynamically inefficient and energy-intensive methods of production. Thus, separated isotopes are a very interesting target for laser photochemistry. The market for separated isotopes other than those used in nuclear power and defense programs, however, is relatively small and may deter large chemical companies from aggressively pursuing methods for laser isotope separation.

Photons as a Feedstock. Since laser generated photons constitute a feedstock to any photo-chemical process, their cost will weigh heavily in the process economics.

The current cost of laser photons from various sources is illustrated in Fig. I.2. A unit of measurement, the Einstein, has been defined as 1 mole or Avogadro's number of photons (6.024×10^{23} photons). The cost of photons is driven primarily by the laser capital cost and not by the cost of electric power to operate the laser. For example, the capital cost of a CO_2 laser suitable for photochemistry work is estimated by Exxon[95] to be no less than $100 per photon watt (1982 $). Although cost figures are somewhat uncertain until actual industrial experience is gained, one can make a crude cost estimate for CO_2 photons to illustrate the major factors involved.

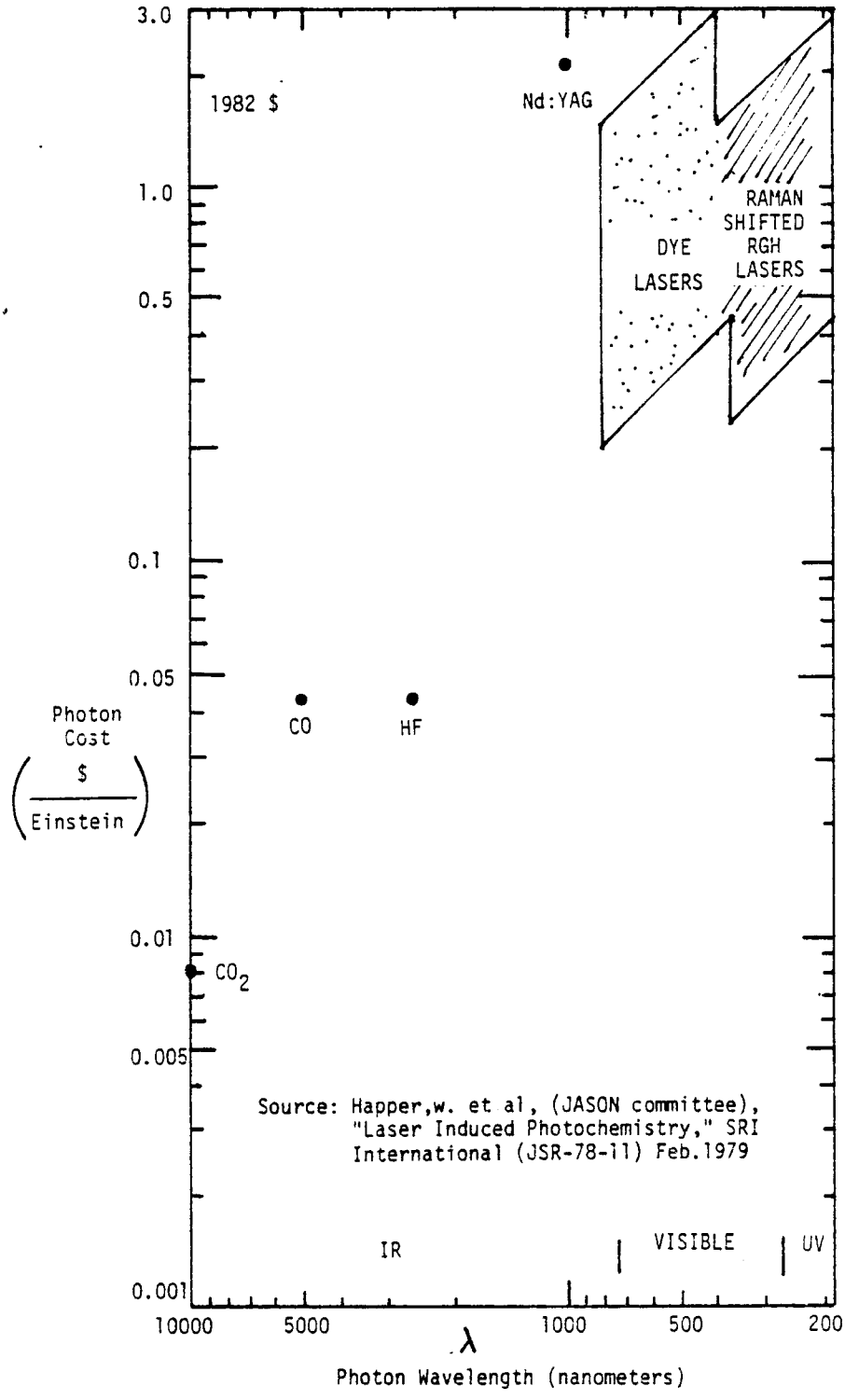


Figure I.2

Cost of Laser Photons as a Function of Photon Wavelength

Consider a 1000 W (photon output) CO_2 laser which operates for 8000 hours per year. Since there are 8760 hours in a year, this corresponds to a 91 percent availability. This laser produces 2.88×10^{10} joules of radiant energy per year. Since a CO_2 photon at a wavelength of 10.6 μm carries 1.88×10^{-20} joules, the laser produces 1.53×10^{30} photons per year or 2.54×10^{6} Einsteins per year. The wall-plug efficiency, i.e., the ratio of light energy output to the input electric energy, of a CO_2 laser can be as high as 20 percent, but efficiencies of large practical lasers are estimated by laser experts to be on the order of 5 percent. Thus, the yearly cost of electrical power for a 5 percent efficient 1 kW laser with 8000 operating hours per year and power costs of \$0.03/kWhr is \$4800 or \$0.0019 per Einstein. Other operating costs, such as maintenance, are, as shown below, likely to be at least as expensive.

At a capital cost of \$100 per photon-watt, the purchase price of the laser will be \$100,000. Assuming amortization over 25 years at an interest rate of 10 percent per annum (capital recovery factor of 11% per year), the annual capital cost is \$0.11 x 100,000 or \$11,000 per year. The capital cost is thus \$0.0043 per Einstein. Maintenance, make-up gas, and labor are roughly estimated to add another \$0.002 per Einstein in operating cost. The total cost of CO_2 photons (in \$ per Einstein) is thus roughly calculated (1982 \$).

Capital Cost	0.004
Maintenance, Labor	0.002
Electric Power	0.002
Total	0.008

While these cost estimates are crude they do illustrate the contributions of both capital and maintenance costs to the molar cost of laser photons. The capital cost of a laser system is dominated by such conventional components as switching circuits, energy storage capacitors, transmission lines, cathodes, gas handling circuits, heat exchangers, space frames, and cabinets. There is no reason to expect any major reduction of capital costs for most of these items, since many of them are conventional components.

The relative cost figures for chemicals and laser photons show very clearly that the cost of an Einstein or g-mol of laser photons is comparable to or exceeds the price of a g-mol of many industrial chemicals. One must also remember that more than one photon may be required to trigger a chemical reaction. This is especially true for CO_2 laser infrared (IR) photons which carry only 0.12 eV or 23 Kcal/g-mol of energy, much less than the energy (40-150 Kcal/g-mol) of most stable chemical bonds. To impart 2 eV to a molecule, an energy comparable to that needed to break several fairly weak chemical bonds in a single molecule seventeen IR photons would have to be absorbed. It is also unreasonable to expect that the IR photons from the CO_2 laser will all be absorbed in quantities of exactly 17 quanta per molecule. Because of attentuation and the temporal and spatial shape (intensity vs. the dimensions and duration) of the laser radiation pulse, some molecules will absorb somewhat more or somewhat less than the proper number of photons needed to trigger the desired chemical reaction. The low unit cost of CO_2 photons compared to visible or ultraviolet photons may therefore be illusory, since only one visible or ultraviolet photon is

required to initiate many reactions of interest, while tens or possibly hundreds of CO_2 photons per molecule are needed for IR triggered reactions.

Other unit cost quantities are useful for describing laser photon costs. Dollars per joule is useful to the process analyst who must deal with engineering calculations. Translating the CO_2 photon cost of \$0.008 per Einstein above to these units would give $\$7 \times 10^{-7}$ per joule of IR energy. Cost per watt of photon power is a common unit; however, its calculation requires information on the nature and repetition rate of the laser energy pulses for the application of interest.

Beyond the cost of the photons, there is an additional aspect of a laser-based process to be considered, the number of product molecules produced per photon, i.e., the quantum yield. From the latter the cost of photons per mole of <u>product</u> can be calculated.

Independent of the type of laser used, the product of a process with a low quantum yield must have an intrinsic value well above, and a volume well below, that of bulk chemicals. This is the reason for the emphasis to date on isotopes for the nuclear industry. There are additional candidates in this cateogory, some of which are mentioned below. In order to consider the laser-based synthesis of a bulk chemical, the quantum yield must be very high.

A simple analysis of the economics of laser photochemistry can be carried out as follows. Introducing the symbols,

C_p = cost of one Einstein of laser photons,

C_1 = other costs for a mole of product, exclusive of photon costs

C_0 = cost of preparation of a mole of product by a conventional process

N = number of photons required to process each product molecule (reciprocal of the quantum yield if the product consists predominantly of molecules capable of undergoing photolysis).

Clearly, a laser photochemical process will only be of interest if the total cost of production with the laser is less than the conventional cost of production, i.e., only if

$$C_1 + NC_P < C_0 .$$

The search for potentially important industrial applications of laser photochemistry is guided by the economic constraints of the above equation. Some obvious implications are:

1. The number N of photons required to process each product molecule should be as small as possible and can be greater or less than one. For example, in multiple photon dissociation of polyatomic molecules (UF_6, SF_6, etc.) by IR lasers, dozens of photons may be absorbed per dissociated molecule. Consequently for multiple quantum infrared chemistry one can hardly expect the number of photons required to effect a chemical reaction to be much less than, e.g., 50. Should it be necessary to use laser photons to process each molecule in the product stream we would then have $N \sim 50$, and the cost C_0 of the product would have to exceed $NC_{ph} = 50 \times \$0.008 = \$0.40$ per g-mol to be of interest, even if the other costs of production C_1 were negligible. This is well above the unit production cost (and price) of most chemicals in large-scale production.

N can be less than 1.0 for those cases in which the product is a substance from which an impurity is being removed. In these cases the product molecule is not the species undergoing a photolytic reaction, rather the impurity that is being photolytically rendered into a form to facilitate its easy removal.

2. Several methods are commonly proposed to make N, the number of photons required to process each product molecule, as small as possible. As mentioned previously, one interesting possibility is to use laser photons to remove trace impurities from a product stream. In such cases the number of photons required per product molecule will be proportional to the concentration of the impurity which is being removed. A photochemical process of this type can be cheaper than an application in which $N \gg 1$ since one need only work on the dilute impurities with the costly laser photons. Essentially one is dealing with a stripping process. The example process to be described and analyzed in this Appendix is in this category.

A photochemical method to purify silane for use in semiconductors has been proposed by Los Alamos National Scientific Laboratory[96] and a similar method to remove H_2S from synthesis gas has been suggested by H. Chen at Lawrence Livermore National Laboratory.[97] Another possibility is the use of laser photons to produce catalytic molecules for use in triggering specific desired reactions. Laser photons have also been proposed as initiators of free radical chain reactions. Convincing examples of the practical advantages of a laser in such processes are lacking.

3. The economic constraints imposed by the above equation are severe. The laser photons alone could add several cents per g-mol to the cost of production of chemicals. This is shown in the earlier Fig. I.1, where optimistic cost estimates for ArF laser (UV) and CO_2 laser (IR) photons are indicated. The use of one or more laser photons per product molecule is therefore economically infeasible in almost all cases except for substances, such as isotopes or specialty chemicals, for which conventional production costs are very high. Most current efforts to find near-term applications of lasers are directed toward utilization of photons where one photon in essence processes many product molecules by removing dilute impurities. Two examples of impurity removal processes are discussed in the next subsection, with one of these applications (laser cleanup of H_2S from synthesis gas) chosen as the example technology for which the methodology presented in Chapters IV through X will be demonstrated.

Promising Applications Involving Elimination of Trace Impurities

Silane Purification

Laser-driven photochemical reactions can be used to selectively remove trace impurities from high purity feedstocks. Silane (SiH_4), an important feedstock for epitaxial growth of silicon crystals used for semiconductor devices, often contains trace amounts of diborane (B_2H_6), arsine (AsH_3), and phosphine (PH_3). These impurities are particularly annoying since they are excellent p- and n-type dopants of silicon. A group at Los Alamos National Scientific Laboratory[98] has suggested that photolysis of silane with ultraviolet lasers, e.g., ArF laser

generated photons at 193 nm, could be used to selectively remove AsH_3, PH_3, and B_2H_6. All of these impurities have much larger photodissociation cross sections than SiH_4, i.e., these molecules have a higher probability of dissociating when exposed to a stream of photons. Preliminary experiments at LASL have demonstrated that the photolysis of silane, which has been intentionally contaminated with AsH_3 and PH_3, produces a white precipitate which includes most of the arsenic and phosphorus impurity along with some silane photofragments. The residual silane is left substantially cleaner by this photolytic step.

Silane purification is an excellent example of the use of laser photons for impurity removal in order to upgrade a high-value product. Each laser photon in effect processes many silane molecules for each impurity molecule with which it really interacts, hence N in the equation in the previous subsection is effectively much less than unity. In spite of its attractiveness, the ultimate economics of silane purification with lasers are not yet clear. Conventional purification techniques utilizing chromatographic columns, for example, are very effective, and the potential for improvement is unknown because of proprietary secrecy.

Laser Cleanup of H_2S from Synthesis Gas

Hydrogen sulfide (H_2S) can be selectively stripped from a synthesis gas (syngas) consisting of CO + H_2 by photolysis using a UV laser. The sulfur thereby generated in the atomic or radical form is irreversibly removed by a metal surface or by polymerization. Removal of sulfur from synthesis gas produced from coal would allow the gas to be used as a

feedstock for organic chemicals (such as methanol) without the destruction of metal or metal oxide catalysts associated with sulfur compound impurities. The laser purification method suggested by Chen, et al.[99] and described and modeled here is a potential practical approach to achieve sulfur impurity levels < 0.1 ppm. This method may have potential industrial significance for extending the lifetime of metal catalysts and scientific feasibility (RD&D Level I) of the method has been accomplished by Chen and coworkers at Lawrence Livermore National Laboratory in California.

Synthesis gas cleanup - process description and chemistry. The process considered is that described in an article by H. L. Chen and C. Borzileri[100] and is here summarized. Synthesis gas (predominantly H_2 and CO), an important chemical feedstock[101] for the synthesis of methanol, methane, glycols, and other hydrocarbons, often contains trace amounts of sulfur compounds (mainly H_2S with some COS and CS_2). These impurities are undesirable since they are extremely reactive with the metallic and metal oxide catalysts used in chemical syntheses. Sulfur poisoning of these catalysts often leads to rapid degradation of catalytic reactivity and a shorter catalyst lifetime. For the copper-based catalysts used in the low pressure synthesis[102],[103] of methanol from synthesis gas, the H_2S impurity level must be kept at the 0.5 ppm level or lower for a catalyst lifetime of one year. Synthesis gas purification below the 1 ppm impurity level is commonly achieved by an effective but rather expensive chemical process using ZnO beds. The laser purification technique described here, if economically and technically feasible, could be used as a direct substitute for this ZnO

process. The conventional precursor scrubbing methods,[104] using chilled polar solvents or active carbon, are retained (and necessary) for the removal of the bulk of the H_2S and other acid gases, initially comprising approximately 13000 ppm, in the synthesis gas stream.

The laser scheme is based on the photodissociation of H_2S[105-107] by either a rare gas-halide (RGH) or a Raman-shifted RGH UV laser:

$$H_2S + h\nu\ (\lambda \cong 210\ nm) \rightarrow H + HS \qquad (1)$$

In the presence of a metal or metal-oxide surface placed in the flow stream, the HS fragment can undergo irreversible surface reactions leaving the sulfur atoms bound as a metal sulfide or deposited as solid polymeric sulfur:

$$HS + M \rightarrow S + M + H \qquad (2)$$

$$HS + M + S \rightarrow M + S_2 + H \qquad (3)$$

where M is a metallic surface or surface-adsorbed species.

There are three scientific issues pertaining to the economics of this purification process. The central spectroscopic issue is that of selectivity or the degree of unwanted laser light absorption by the synthesis gas (particularly CO) and impurities (such as C_2H_4, CH_3OH, O_2) whose removal is not beneficial to extending catalyst lifetimes. These impurities are either intrinsic to the actual gasification process or are introduced during the prescrubbing of H_2S (from 13000 ppm to the 1 to 10 ppm level) by conventional precursor sulfur removal methods. The other two issues of equal importance are the quantum yield for dissociation and deleterious effects due to post-photolysis phenomena. It is also important to demonstrate efficient conversion of the HS fragments to metal sulfide or polymeric sulfur.

To determine whether or not H_2S could be selectively dissociated with a UV laser in the presence of synthesis gas, absolute absorption cross sections have been measured[108] for the synthesis gas over 190 to 250 nm with ArF and KrF RGH type lasers and a frequency-shifted dye laser.

UV absorption data suggest that a spectroscopic selectivity, i.e., the ratio of the absorption cross sections ($\sigma_{H_2S}/\sigma_{syn}$) of 10^7 is feasible if one uses a laser in the 210 to 220 nm wavelength region. A frequency-shifted ArF laser[109] (at 210 nm) appears to be the best candidate. Other types of RGH laser systems such as a frequency-shifted KrF laser[110] (at 225 nm) or a KrCl laser (at 220 nm) would also serve the purpose.

To determine the overall quantum yield of H_2S removal, including post-photolysis effects, experiments were performed by Chen[111] and coworkers with H_2S at various synthesis gas densities. The objective of these experiments was to determine the ratio of

$$\frac{[H_2S] \text{ removed from synthesis gas}}{[h\nu] \text{ absorbed by the } H_2S \text{ molecules}} .$$

The results show that the quantum yield of H_2S removal turns out to be near unity at low pressure (~ 10 torr) and decreases to roughly 0.4 at 1 atm. The partial pressure of H_2S for these experiments was kept at 2 millitorr.

Little is known about the reactivity of the HS radical with metal surfaces. Low density photolysis data seem to indicate that reactions (2) and (3) are quite fast. At low synthesis gas density, most of the HS radicals initially produced by the photolysis pulse were transformed into metal sulfide or polymeric sulfur and hence removed from the gas stream.

Additional HS radicals might also have been generated by reaction between H_2S and H atoms on the collector surface.

$$H_2S + H \rightarrow H_2 + HS + 12 \text{ kcal/mole} . \quad (4)$$

This is consistent with Chen's experimental findings[112] where the measured quantum yield of H_2S removal is near unity at the low density conditions. The smaller quantum yield observed at higher synthesis gas densities may result from the post-photolysis recombination reaction of HS radicals prior to their polymerization on the metal surface:

$$HS + HS \rightarrow H_2S + S + 11 \text{ kcal/mole} . \quad (5)$$

Preliminary Economic Feasibility Analysis at Lawrence Livermore National Laboratory

Based on the spectroscopic selectivity and quantum yield for sulfur removal, preliminary cost analysis for an H_2S cleanup process has been made for a process utilizing a frequency-shifted ArF laser operating at a 210-nm wavelength. The estimated laser purification costs for various H_2S concentrations in a syngas feedstock are listed in Table I.1 compiled by Chen et al.[113] at Livermore. Clearly, the projected purification cost is a function of many parameters such as spectroscopic selectivity, quantum efficiency, laser fluence, laser efficiency, frequency conversion efficiency, laser-equipment capital, replacement and repair costs, and photon utilization efficiency. The values of the parameters used in this reference analysis are also given in Table I.1. For comparison, the costs for a conventional chemical method using ZnO at 350°C are also shown. The above preliminary analysis shows that laser purification appears to be uneconomic for an initial H_2S level much greater than 1 ppm. However, at an initial H_2S impurity level of

Table I.1

Livermore Reference Photochemical Syngas Cleanup Process
Including Comparison with ZnO Purification Method

H_2S Impurity Levels	Laser Purification* ($/mol of S removed) (1980$)	ZnO Purification ($/mol of S removed) (1980$)		
		Bulk Gas** Heating Cost	ZnO Material Cost	ZnO Unit*** Capital Charges
10 ppm → 1 ppm	<10	2	0.5	N/A
1 ppm → 0.1 ppm	10 to 20	20	3	20
0.1 ppm → <0..5 ppm	<100	200	~ 15	N/A

*Calculated for:

Photon cost = 1$/mol; mainly capital and maintenance changes of laser
Laser photon flux = 0.5 j/cm^2, quantum yield of H_2S removal = 0.5,
Raman shifting efficiency = 0.5
Photon utilization efficiency = 0.5 (for 10 ppm, ℓ = 10 m)
= 0.35 (1 ppm, ℓ = 10^2 m)
= 0.04 (0.1 ppm, ℓ = 10^2 m)

**Heat provided by synthesis gas at 7 mil/kWhr, negligible if one uses waste heat

***25% of process unit investment

N/A: data not available

Source: Chen, H. L., et al., IEEE J. of Quantuam Electronics, Vo. QE-16, No. 11, (Nov. 1980).

1 ppm or lower, the above analysis infers that the laser process may become more competitive than the conventional ZnO process. For the catalytic synthesis of methanol from syngas ($CO + 2H_2 \rightarrow CH_3OH$), the cost increase due to the addition of the laser purification process is projected to amount to roughly 1 percent of the current methanol chemical value ($175/ton). The costs for the laser process are due mainly to the capital and maintenance charges of the laser system. On the other hand, the cost for the chemical method using a ZnO guard bed is due mostly to the capital cost for the ZnO reactor and the operating costs for bulk gas heating required for promoting the ZnO/H_2S reaction on the ZnO pellet surfaces.

This early estimate is somewhat crude and represents preliminary back-of-the-envelope type calculations rather than a detailed design and cost estimate. Many costs such as auxiliaries, balance of plant, engineering, contingency, labor, and replacement have been ignored. This preliminary cost, however, does appear sufficiently attractive to warrant further economic evaluation studies. This effort is described in the following subsections. It is presumed that this process meets the conditions for applicability of this methodology as set forth in Chapter IV.

Performance and Design Analysis

In order to verify these preliminary Livermore analyses[114] and provide a basis for the economic methodology to be presented in the next section, it is necessary to define a point design or reference case and construct parametric performance and economic models for the photolytic

syngas cleanup method. Evaluation of the construction of the process assessment model will follow the methodology outlined in Chapters V and VI.

Process Definition

The sulfur removal step is one step of many on the route from a raw material (coal in this case) to a finished product (methanol). The unit costs associated with methanol production include the cost of synthesis gas, which in turn depends on the price of coal; the operating costs of the gasification technology used; the desulfurization cost, which is the main process step considered here, and the operating costs of catalytic methanol synthesis. In order to properly consider desulfurization alternatives, it is necessary to select and fix the overall framework in which the alternatives will operate. Chen and Borzileri[115] reference an EPRI study[116] concerning the production of methanol as a possible fuel for peak shaving applications in electric power generation. The latter paper includes a methanol synthesis flow sheet which provides a suitable basis for insertion of a photolytic process to replace conventional ZnO bed sulfur removal. In the EPRI report the authors consider the economic incentives for developing a sulfur-tolerant catalyst for the methanol synthesis step as an alternative to sulfur removal. The economics of ten conceptual methanol production schemes, with varying levels of H_2S allowed in the synthesis gas feed, were reviewed. In all cases the methanol synthesis was based on Chem Systems Corporation's liquid phase process operating at near 80 atm. The lowest cost methanol synthesis route was chosen as the framework for evaluating the photochemical sulfur removal process. A schematic flow diagram for the synthesis

gas route to methanol is shown in Fig. I.3 and the steps are as follows:

1. Raw synthesis gas (syngas) is produced in a coal gasifier of the Lurgi or Texaco type at an H_2/CO ratio of 2. The gas is discharged at 465 psia (31.6 atm or 24,000 torr) and 120°F (322K) and is assumed free of tar and ash.

2. The bulk of the sulfur bearing or acid gases, at a concentration of 13,000 ppm S in the syngas, is removed via a high pressure H_2S absorption process such as the Rectisol process or a Benfield hot K_2CO_3 scrubbing process. The H_2S rich stream from this unit operation is fed to a Claus type sulfur recovery plant after these precursor steps. The cleaned synthesis gas has a concentration of 5 to 100 ppm H_2S, depending on the size and efficiency of the bulk sulfur removal equipment.

3. Long life for the methanol production catalyst is ensured by further lowering the sulfur content in the syngas stream to 0.1 ppm or less. The conventional technology utilizes ZnO catalyst beds operating at 448°F (404K). If a sulfur tolerant catalyst for methanol production or a photochemical method for sulfur removal were available and proved economical, this expensive catalytic step could be eliminated or replaced.

4. Methanol synthesis, via the reaction $H_2 + CO \rightarrow CH_2OH$, utilizes the Chem Systems approach in which a fluidized catalyst is suspended in an inert liquid phase for efficient removal of the heat of reaction. Nearly complete stoichiometric conversion of the 2/1 H_2/CO mixture is achieved by recycling unreacted syngas back to the reactor and purging any CO_2 produced. The reaction takes place at 448°F (404K) and a

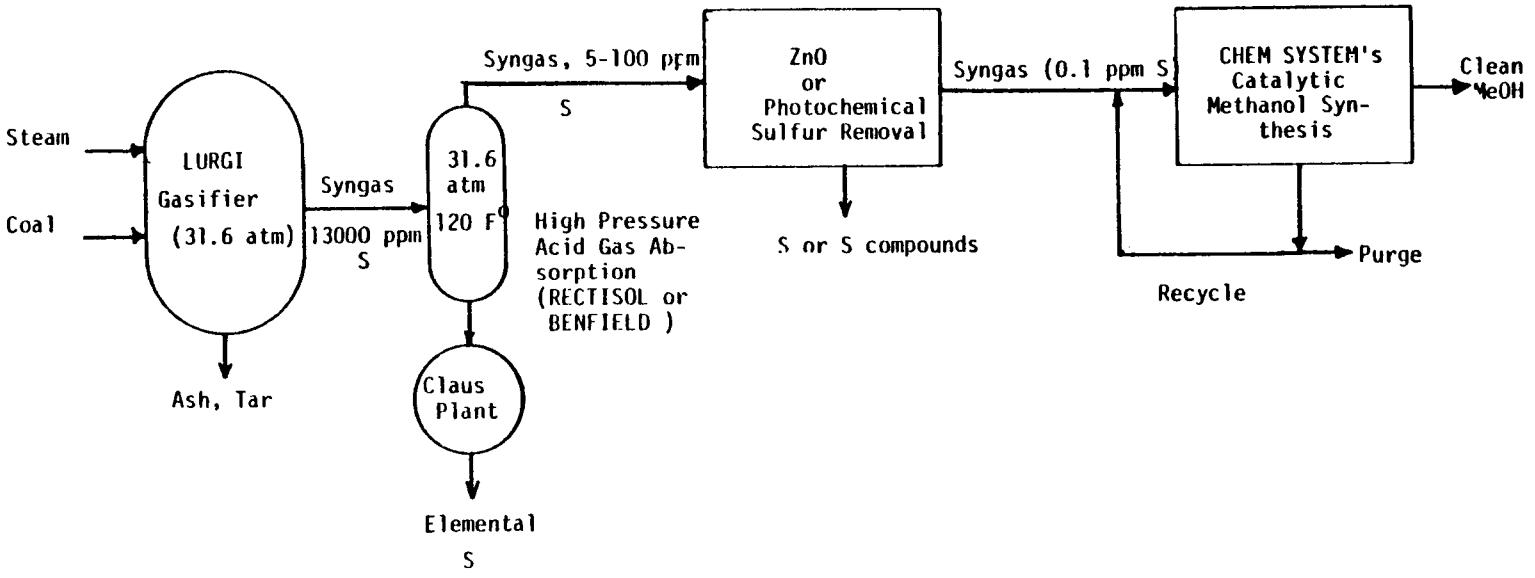


Figure I.3

Synthesis Gas Route to Methanol Incorporating
Sulfur Removal Steps

pressure of 1120 psia (76.2 atm or 57,900 torr). The alcohol product so synthesized is nearly free of sulfur and suitable for synthesis into other chemicals or as a fuel. For use as a fuel the level of impurities is not critical. The methanol plant here considered produces 76 tons per hour, requiring the processing of 4.8×10^{10} standard cubic feet of synthesis gas per year.

Now that the task and purpose for low concentration removal have been defined, one must set forth a few assumptions on the baseline photochemical process itself.

1. The photolytic syngas cleanup facility and its associated support facilities will be costed as an add-on facility to an existing methanol plant.

2. The facility will be designed to handle the 4.8×10^{10} standard cubic feet per year of syngas contaminated with 5 ppm of H_2S. The exiting stream will contain 0.1 ppm H_2S or less (a decontamination factor of 50).

3. A single pass or single stage photolysis process will be used. Each slug of gas passing the laser beam will see only one burst of photons. Recycle and/or multistage photolytic reactors are possible, but are not considered here.

4. Non-H_2S constituents of the syngas stream will be assumed to have a composite UV absorption cross-section sufficiently small that the syngas is not heated enough to cause sudden gas expansion in the reaction or irradiation zone.

5. Sulfur collection will be effected by the layers of metal screens with small enough mesh that HS fragments will strike these

surfaces before colliding with other HS fragments.

6. As will be explained in a later subsection, a photolysis process of this type must operate at low pressure in order to prevent HS-HS and HS-H collisional recombination immediately after photolysis. Both the upstream syngas production unit and the downstream methanol reactor, however, operate at pressures at least an order of magnitude higher. For this reason the syngas must be reduced in pressure, photolytically cleaned, and raised in pressure. A power recovery system is incorporated to reduce the energy loss in these steps. Figure I.4 depicts the photolysis system and its necessary support steps.

Other assumptions are made throughout the analysis and will be explained as the model is presented. Actual FORTRAN coding for the model is given in Appendix J and a block diagram of the SUBROUTINES is shown in Fig. I.5. Part of the performance and design analysis task is the calculation of a base case process design and a subsequent cost estimate. Since an actual design and cost estimate was not available from an engineering group, the author used appropriate portions of the process productivity model to derive his own appropriate design and cost estimate. Later in this Appendix the base case and its associated parameters will be presented. The next subsection describes development of the process performance model.

The Process Performance Module

For this particular application the desired performance or productivity is a fixed entity, i.e., decontamination of 76 tons/hour of a 5 ppm H_2S syngas stream by a factor of 50. Given a set of input performance parameters, the model must calculate the process equipment,

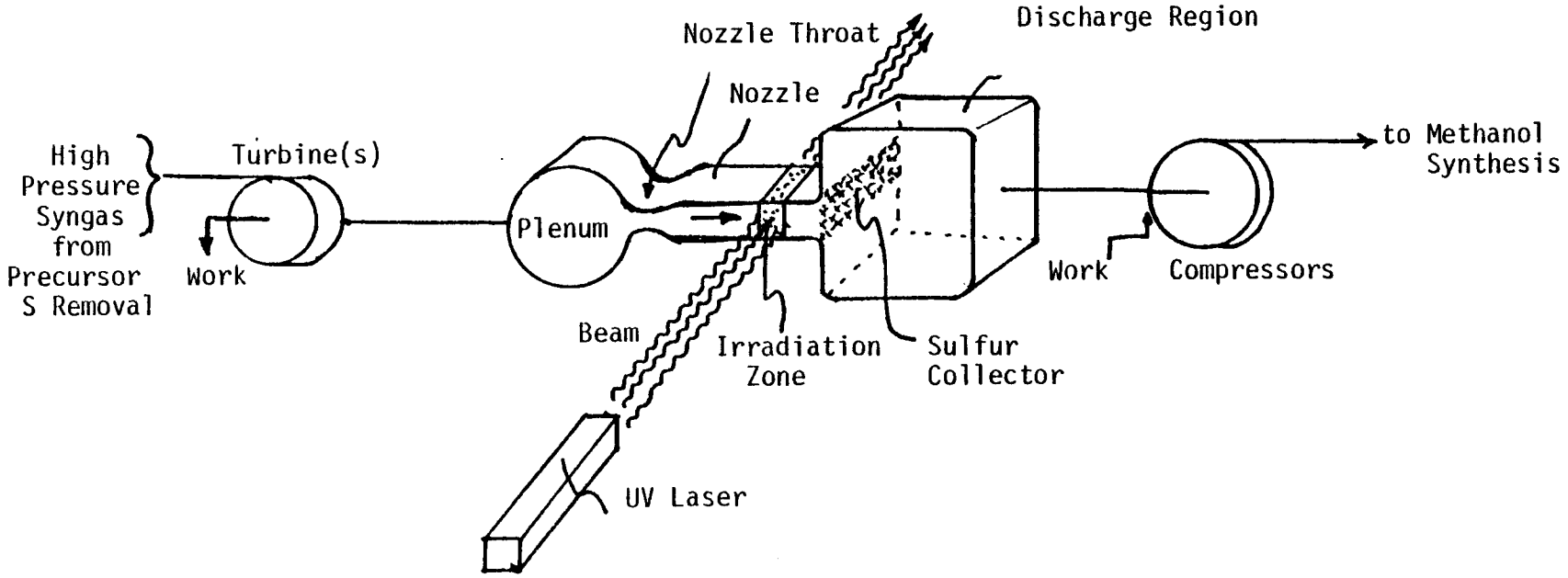


Figure I.4

Schematic: Photochemical Removal of Sulfur
from Synthesis Gas

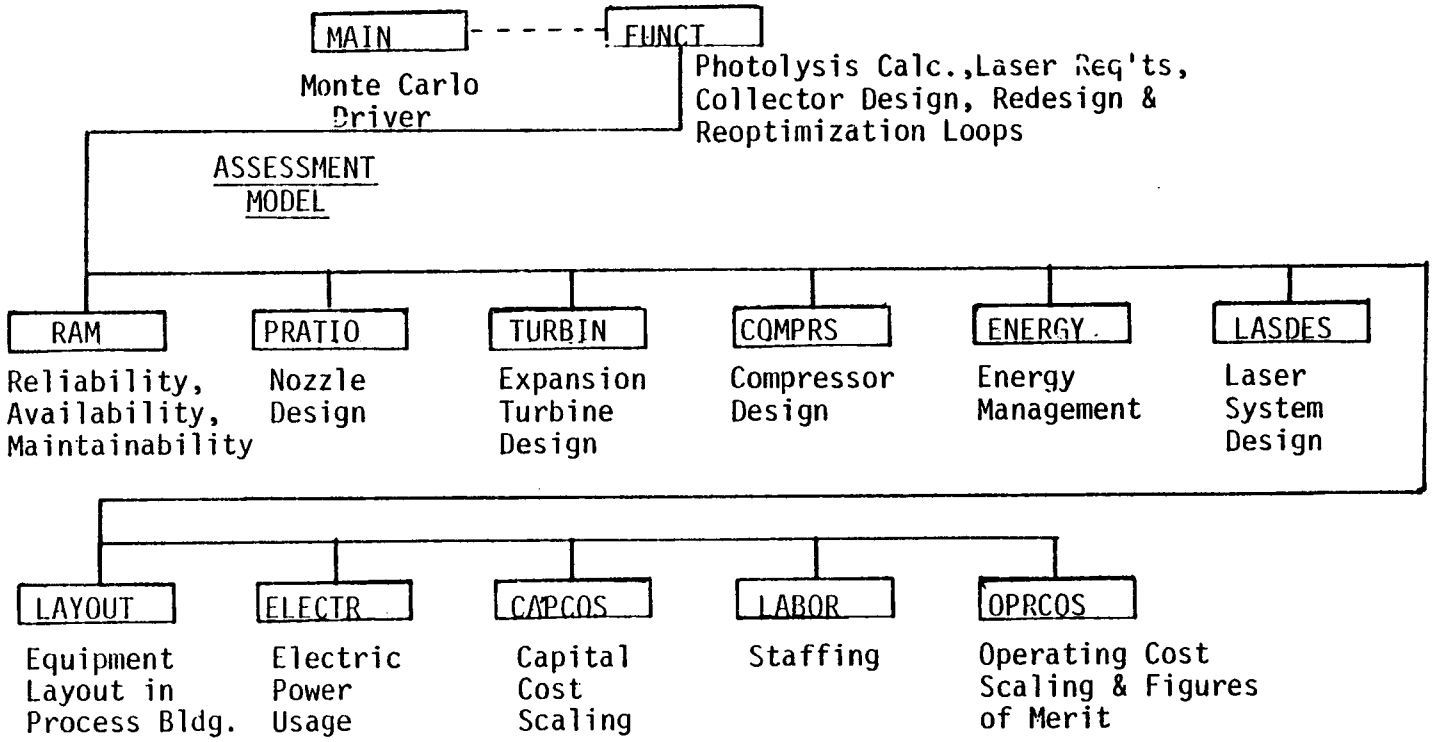


Figure I.5

Structure of Assessment Model

energy, laser, and flow requirements needed to maintain these performance specifications. The heart of the productivity model is the photolysis model, a rate equation treatment of the interaction of intense laser light and H_2S molecules. This photolysis model was constructed with the assistance of D. F. Starr.[117]

Calculation of the photolytic yield: The photolytic yield or cut is the fraction of the H_2S molecules in the volume bounded by the gas flow and the laser beam (i.e., the irradiation zone shown in Fig. I.4) which is dissociated into H and HS photofragments. The variables which determine the photolytic cut are the density of H_2S in the irradiation zone, ρ_{H_2S}; the absorption cross section, σ_{H_2S}; the laser beam fluence or number of photons per cross sectional area of laser beam, ϕ; and the irradiation zone length, ℓ. Assuming perfect selectivity, a reasonable assumption for this process where the measured selectivity is 10^7 or more, the following derivation is presented.

Consider an optically thin slab of irradiation zone of cross sectional area A and thickness $\Delta\ell$ as shown in Fig. I.6.

The number of photons absorbed = $[\phi(\ell) - \phi(\ell+\Delta\ell)]A$

where $\phi(\ell)$ is the laser beam photon fluence at ℓ.

For a thin slab, typical Beer's Law absorption can be assumed; and the number of H_2S molecules dissociated can be represented by:

$$\rho_{H_2S}[1 - e^{-\sigma_{H_2S}\phi(\ell)}]A\ \Delta\ell,$$

where:

ρ_{H_2S} is the H_2S density in molecules/cm^3

σ_{H_2S} is the H_2S absorption cross section (for UV) in cm^2

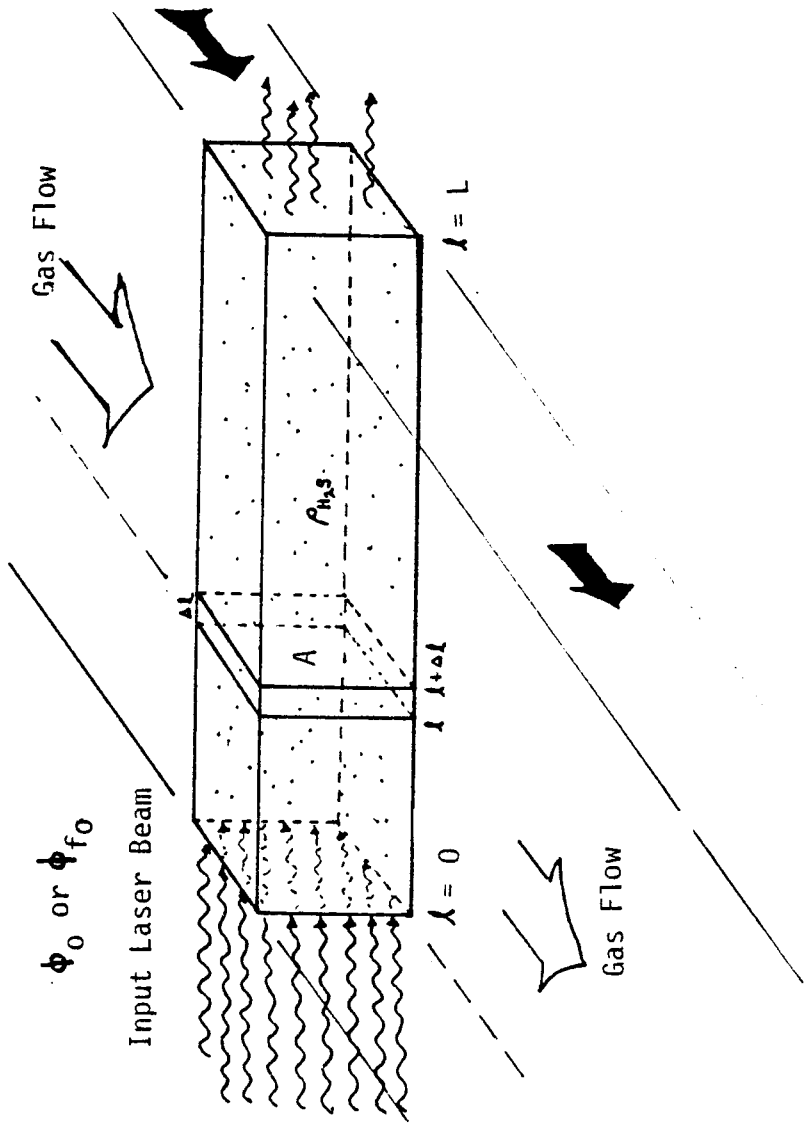


Figure I.6

Interaction Zone Geometry

$\phi(\ell)$ is the laser photon fluence in photons/cm^2, which is directly proportional to the energy fluence, i.e., joules per cm^2

A is the laser beam cross sectional area in cm^2

ℓ is the irradiation zone length in cm.

For an infinitely thin slab, $\Delta\ell \to 0$, and by the definition of a derivative:

$$\frac{d\phi}{d\ell} = -\rho_{H_2S}\left[1 - e^{-\sigma_{H_2S}\phi(\ell)}\right] . \tag{7}$$

Integrating:

$$\frac{d\phi(\ell)}{\left[1 - e^{\sigma_{H_2S}\phi(\ell)}\right]} = -\rho_{H_2S}d\ell \tag{8}$$

$$\int_{\phi(\ell=0)}^{\phi(\ell=L)} \frac{d\phi}{\left[1 - e^{-\sigma_{H_2S}\phi(\ell)}\right]} = -\rho_{H_2S}L \tag{9}$$

If $x = \sigma_{H_2S}\phi$,

$$\int_{\sigma_{H_2S}\phi(\ell=1)}^{\sigma_{H_2S}\phi(\ell=L)} \frac{dx}{1-e^{-x}} = -\sigma_{H_2S}\rho_{H_2S}\,L \tag{10}$$

$$\int \frac{dx}{1-e^{-x}} = \int \frac{e^x dx}{e^x-1} = \int \frac{dU}{U} \quad \text{where } U = e^x-1 \tag{11}$$

$$= \ell n(U) = \ell n(e^x - 1) \tag{12}$$

Therefore (dropping the subscript H_2S on σ and ρ to simplify notation),

$$-\sigma\rho L = \ell n\left[e^{\sigma\phi(\ell=L)} - 1\right] - \ell n\left[e^{\sigma\phi(\ell=0)} - 1\right] , \tag{13}$$

and

$$\frac{e^{\sigma\phi(\ell=L)} - 1}{e^{\sigma\phi(\ell=0)} - 1} = e^{-\sigma\rho L} . \tag{14}$$

If the yield or photolytic cut is defined as $\theta(\ell) = 1\text{-}e^{-\sigma\phi(\ell)}$, i.e., the extent of photon absorption, and $\phi_0 = \phi(\ell=0)$, $\phi(\ell) = \phi(\ell=L)$, the cut at any ℓ can be derived in terms of the input beam fluence at $\ell = 0$.

$$e^{\sigma\phi(\ell)} - 1 = e^{-\sigma\rho\ell}(e^{\sigma\phi_0} - 1) \tag{15}$$

$$e^{\sigma\phi(\ell)} = 1 + e^{-\sigma\rho\ell}(e^{\sigma\phi_0} - 1) \tag{16}$$

$$\theta(\ell) = 1 - e^{-\sigma\phi(\ell)} = 1 - \frac{1}{1 + e^{-\sigma\rho\ell}(e^{\sigma\phi_0} - 1)} \tag{17}$$

$$\theta(\ell) = \frac{e^{-\sigma\rho\ell}(e^{\sigma\phi_0} - 1)}{1 + e^{-\sigma\rho\ell}(e^{\sigma\phi_0} - 1)} \tag{18}$$

For the calculation of this overall yield, the photolytic cut must be averaged over the irradiation zone length L:

$$\theta_{ave} = \frac{1}{L}\int_0^L \theta(\ell)d\ell = \frac{1}{L}\int_0^L \frac{e^{-\sigma\rho\ell}(e^{\sigma\phi_0} - 1)d\ell}{1 + e^{-\sigma\rho\ell}(e^{\sigma\phi_0} - 1)} . \tag{20}$$

$$\theta_{ave} = \frac{-1}{\sigma\rho L}\int_0^L \frac{[-\sigma\rho\ell^{-\sigma\rho\ell}(e^{\sigma\phi_0} - 1)]d\ell}{1 + e^{-\sigma\rho\ell}(e^{\sigma\phi_0} - 1)} \tag{21}$$

$$\theta_{ave} = \frac{-1}{\sigma\rho L}\left[\ell n\ (1 + e^{-\sigma\rho\ell}(e^{\sigma\phi_0} - 1))\right]_0^L \tag{22}$$

$$\theta_{ave} = \left(\frac{-1}{\sigma\rho L}\right)\ell n\left(\frac{1 + e^{-\sigma\rho L}(e^{\sigma\phi_0} - 1)}{e^{\sigma\phi_0}}\right) . \tag{23}$$

Even for a short irradiation zone, there is a limitation on the photolytic cut which can be obtained for a given ϕ_0, σ, and ρ. This limiting

cut is useful for irradiation zone and laser design calculations and is calculated as follows:

For a constant σ and ρ, let $Z = \sigma\rho L$. Letting $L \to 0$, therefore $Z \to 0$. Taking Equation (23) in terms of Z, and the fact that $1 - x \approx e^{-x}$ as $Z \to 0$:

$$\lim_{Z\to 0} \theta = \lim_{Z\to 0} \left[-\frac{1}{Z} \ln\left(\frac{1 + e^{-Z}(e^{\sigma\phi_o} - 1)}{e^{\sigma\phi_o}}\right)\right] \tag{24}$$

$$= \lim_{Z\to 0} \left[-\frac{1}{Z} \ln\left(\frac{1 + (1-Z)(e^{\sigma\phi_o} - 1)}{e^{\sigma\phi_o}}\right)\right] \tag{25}$$

$$= -\frac{1}{Z} \ln\left(\frac{e^{\sigma\phi_o}\,(1 - Z + Ze^{-\sigma\phi_o})}{e^{\sigma\phi_o}}\right) \tag{26}$$

$$= -\frac{1}{Z} \ln\left(1 - Z(1 - e^{-\sigma\phi_o})\right) \tag{27}$$

$$= -\frac{1}{Z} \left(-Z(1 - e^{-\sigma\phi_o})\right) \tag{28}$$

$$\theta_{lim} = 1 - e^{-\sigma\phi_o} \,. \tag{29}$$

The quantity ρ_{H_2S} is calculated via the perfect gas law from the H_2S concentration, the total synthesis gas pressure, the temperature, and Avogadro's Number:

$$\rho_{H_2S} = \frac{PN_{avo}}{RT}\left(\frac{P_{MIL}}{10^6}\right) \,, \tag{30}$$

where:

P = total synthesis gas pressure (in torr or mmHg)

R = gas constant (62,361 torr·cm^3/g·mole·K)

T = absolute temperature of synthesis gas (K)

P_{MIL} = H_2S concentration in parts per million

N_{avo} = Avogadro's Number (6.024×10^{23} molecules/g.mole).

The photon fluence term ϕ_o, along with the laser frequency, λ, can be used to calculate the energy deposited per cross-sectional area of laser beam or energy fluence, ϕ_{fo}, as follows:

$$\phi_{fo} = \phi_o hc/\lambda \tag{31}$$

where:

ϕ_{fo} = energy fluence in joules/cm^2

h = Planck's constant (6.63×10^{-34} joule-sec)

c = speed of light (3.0×10^{10} cm/sec)

λ = laser light wavelength (cm).

The initial fluence, ϕ_{fo}, is a key variable required for the design of a laser system.

Now that the photolytic yield or cut, θ_{ph}, has been determined by the photon/matter interactions above, the collector or post-photolysis chemistry must be examined.

Post-photolysis chemistry. The desired post-photolysis reactions are the surface reactions of HS photofragments with a metal or metal oxide surface placed in the flow stream:

$$HS + M \rightarrow M\text{-}S + H \tag{32}$$

$$HS + M\text{-}S \rightarrow M\text{-}S_2 + H \tag{33}$$

$$H_2S + H \rightarrow H_2 + HS \tag{34}$$

where the dash designates bound quantities and M is a metallic surface or surface adsorbed species. Experimental data indicate that the first

two reactions are quite fast and that at low density (2 millitorr partial pressure of H_2S) most HS can be easily removed from the gas stream. As the H_2S partial pressure is increased, however, the following recombination reaction may undo part of the photolysis:

$$HS + HS \rightarrow H_2S + S \ . \qquad (35)$$

If this reaction were to dominate completely the kinetics of post-photolysis the maximum recombination yield would be 0.5, since elemental sulfur itself is a product. In order to achieve a high quantum yield, i.e., close to 1.0, one must minimize the opportunity for HS-HS collision to ensure that reactions (32) through (34) above will predominate. The collector placed in the postphotolysis flow stream must intercept the HS fragments before they have a chance to collide. The distance traveled by an HS fragment from its birth to a collector surface must be less than a mean free path for an HS-HS collision. Figure I.7 shows how the post-photolysis quantum yield is expected to vary with H_2S partial pressure.

The post-photolysis quantum yield is important and is mentioned at this point because of its effect on the overall cut required to obtain the desired factor of 50 decontamination. The overall cut is expressed as:

$$\theta_{tot} = \theta_{ave}\ \theta_{pp}$$

where:

θ_{tot} = the total or stage cut or total yield actually achieved in the collector, i.e., the actual fraction of the S atoms in the syngas collected

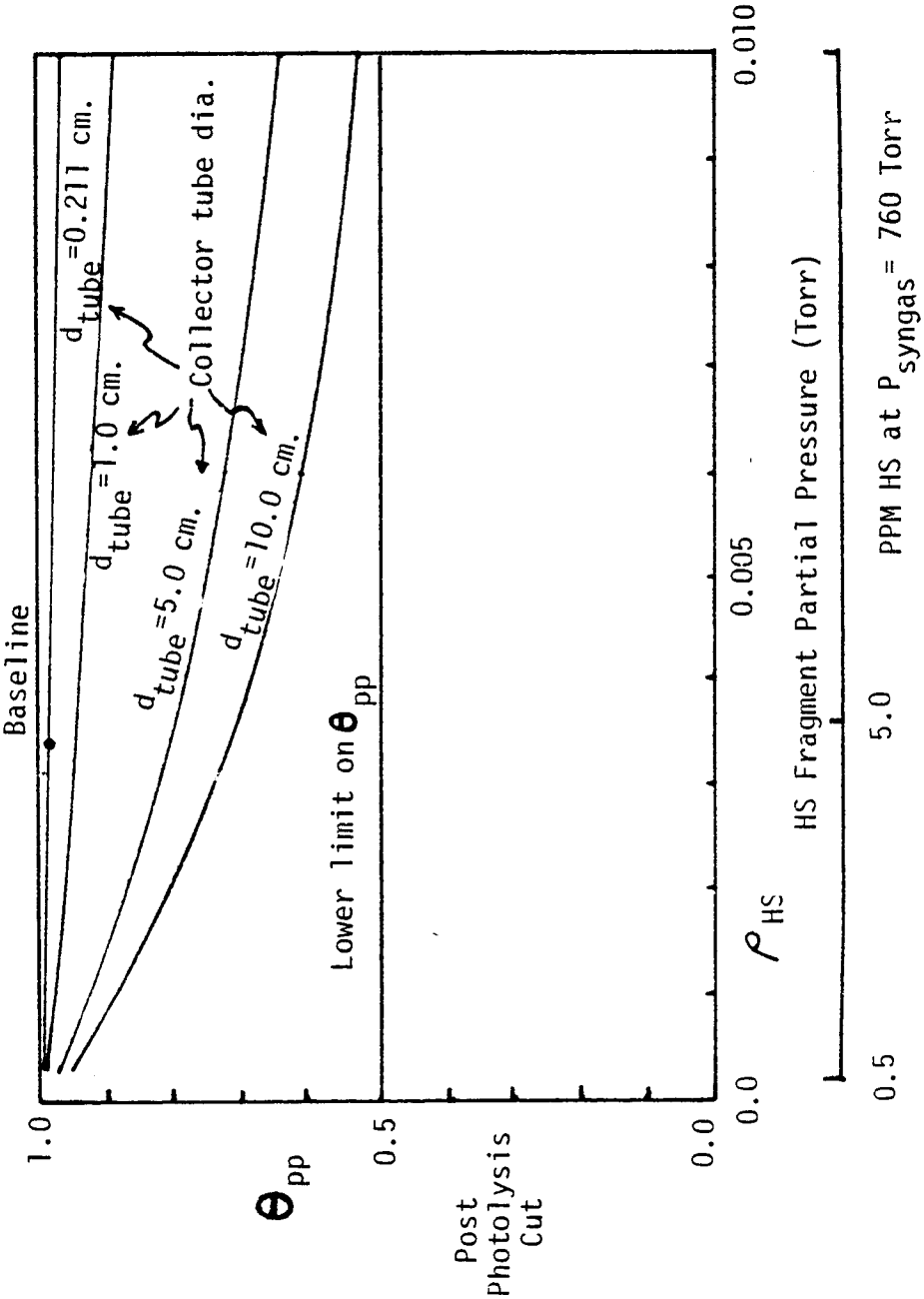


Figure I.7

Post-Photolysis Cut as a Function of HS Fragment Partial Pressure

θ_{ave} = the average fraction of the H_2S dissociated by the laser (a function of ϕ_o, ρ_{H_2S}, σ_{H_2S}, and L)

θ_{pp} = the post-photolysis quantum yield achieved in the collector, i.e., the fraction of HS photo-fragments adhering to a collector and not recombining (a function of the HS fragment partial pressure, the reaction rate for Equation 35, and the collector pore size).

For the decontamination task defined, θ_{tot} must be greater than or equal to 0.98.

Performance model requirements. In order to initiate the photophysics model, an initial estimate for the photon flux or fluence is needed before Equations (18), (23), and (29) can be accessed. Since the limiting cut, θ_{lim}, is a function of fluence, ϕf_o, only (for a given σ_{H_2S}) a ϕf_o can be calculated by inversion of Equation (29) and setting θ_{lim} equal to 0.99. This ϕf_o value is a first guess for use in Equation (23) for calculation of θ_{ave}. This calculation requires a value for the gas density, ρ, and the irradiation zone length, L. The irradiation zone length depends on the cross sectional area perpendicular to the flow direction of the nozzle, and is calculated in the aerodynamic nozzle design part of the model to be described below. The value of θ_{ave} from Equation (23) and ϕf_o, L, and ρ is always slightly smaller than the limiting cut, θ_{lim}. To calculate the total cut, θ_{tot}, the post-photolysis cut, θ_{pp}, must also be estimated. The HS fragment density, ρ_{HS}, needed for the calculation of θ_{pp} is a function of θ_{ave}. This ρ_{HS} value along with the collector pore size can be used to obtain θ_{pp} from Fig. I.7. The collector design algorithms used to generate

Fig. I.7 are deferred to the process design module description to avoid repetition here. A collector pore size is picked such that θ_{pp} will be greater than the square root of θ_{lim}. This is done to fulfill the requirement that the product $\theta_{ave}\ \theta_{pp} \simeq \theta_{tot} \simeq 0.98$. If the resulting total cut, θ_{tot}, is less than 0.98, ϕ_{fo} is increased and the entire sequence repeated until the product $\theta_{ave}\ \theta_{pp}$ is greater than or equal to 0.98. Several iterations may be required. Figure I.8 shows the logic for this calculation in DTFR block diagram form. Once that the required laser energy fluence, ϕ_{fo}, for this task has been calculated, the design equation and hardware requirements for the actual laser system can be discussed.

Deviation/Transfer Function/Response Structure of Performance and Design Modules Including Redesign and Reoptimization Capabilities

Figure I.8 shows that the collector tube diameter and the laser fluence are used to redesign and reoptimize the process. One wishes to minimize the laser fluence ϕ_{fo} for a given set of input conditions. By doing so, the total annualized costs are also reduced. This statement can be made since it is known that the laser system is by far the largest driver of the capital and operating costs. Any reduction in ϕ_{fo} results in less laser power required and less electrical energy to run the laser. An iteration loop is used to calculate the lowest ϕ_{fo} that allows the total cut, θ_{tot}, to be greater than or equal to 0.98. The collector is also redesigned such that the pore size will allow this same θ_{tot} goal. A θ_{tot} of 0.98 assures that the performance requirement of a decontamination factor of 50 can be met.

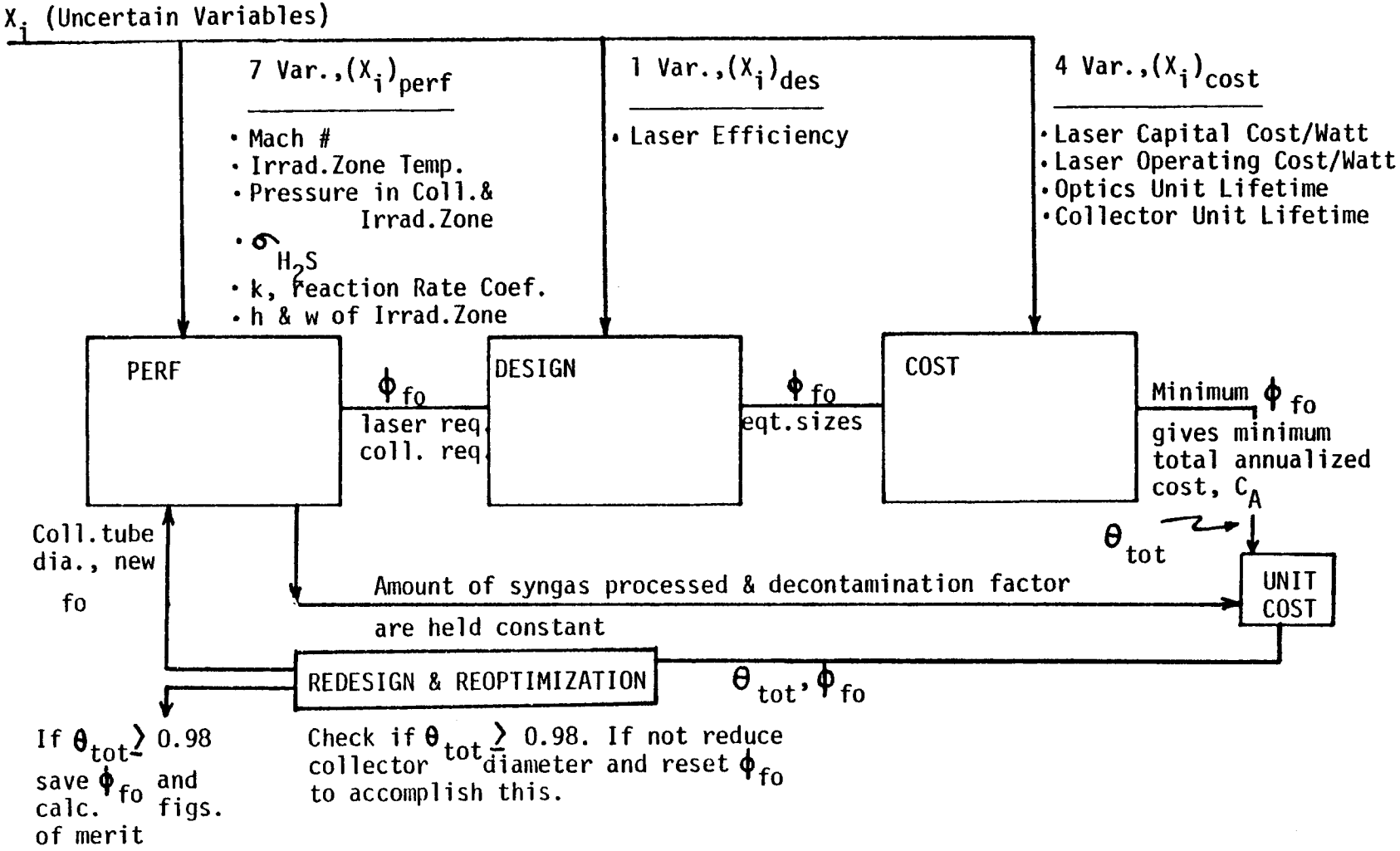


Figure I.8

Structure of Syngas Cleanup Assessment Model

The Process Design and Equipment Sizing Module

The above step considered the theory and requirements for H_2S photolysis in detail. The design model, which also invokes significant process science, calculates the auxiliary equipment sizes and energy requirements necessary to maintain the conditions necessary for photolysis. The problem of syngas conditioning will be handled by an aerodynamic model, collector design by a collisional model, and laser system design by a simple scale-up model in this step.

The aerodynamic model. Design criteria for the laser-discharge cavity limit the aperture size, in cross sectional area, of the output beam to only a few square centimeters. From the configuration of the gas-beam system, as shown in Fig. I.6, the need for a long, narrow flow channel or nozzle is indicated. The nozzle height is closely related to the laser beam height, typically in the 0.5 to 3.0 cm range, and the desired syngas pressure in the irradiation zone. The nozzle length is also the path length of the laser beam through the gas, typically on the order of few meters. Figure I.9 shows the nozzle configuration. The fact that a long, narrow slit is needed for gas flow mandates a high-speed flow to process the desired volumetric flow of syngas. By using a small nozzle throat height the velocity in the irradiation zone slightly downstream of the throat can be made supersonic, up to a dimensionless factor, F_{RM}, times the Mach number, where:

$$M = \text{the Mach number} = v/v_{sonic} \tag{37}$$

and

$$F_{RM} = \sqrt{2}/\sqrt{\gamma-1} \tag{38}$$

where γ is the heat capacity ratio for the syngas.

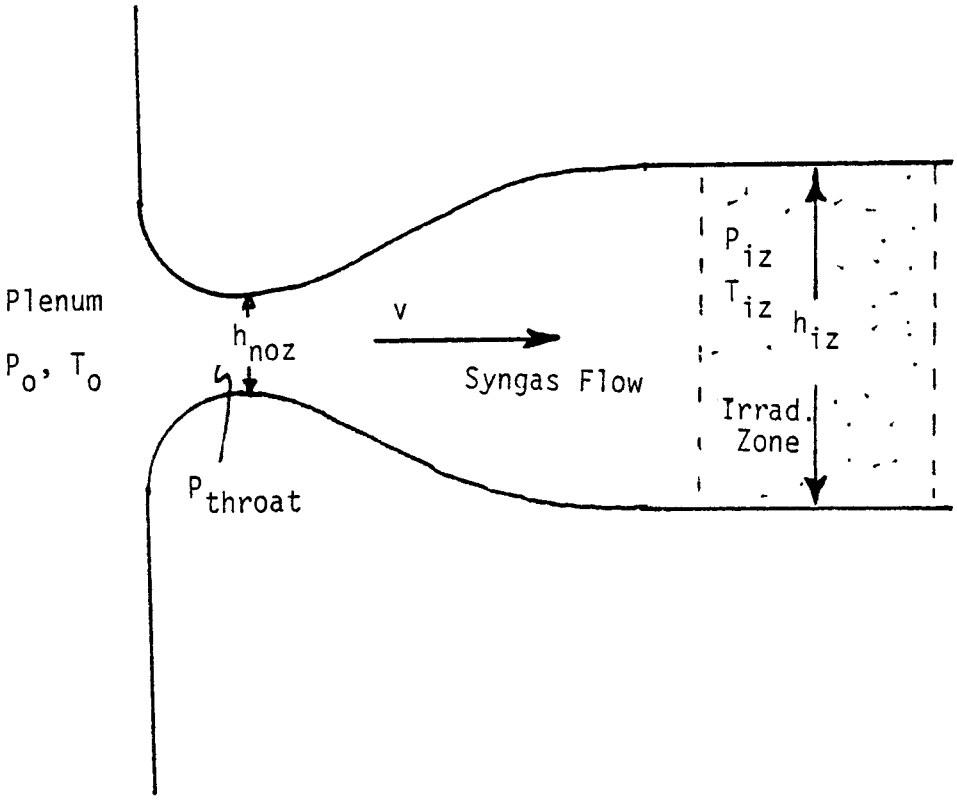


Figure I.9

Nozzle Configuration

In order to obtain a supersonic flow downstream, the plenum pressure upstream of the nozzle throat must equal or exceed that calculated from the critical pressure ratio,

$$r_{cp} = \frac{P_{throat}}{P_o} = \left[\frac{2}{(\gamma+1)}\right]^{(\gamma/\gamma-1)} \tag{39}$$

where:

P_{throat} = the syngas pressure in the nozzle throat (same units as P_o)

P_o = the pressure in the plenum upstream of the nozzle

γ = the heat capacity ratio, C_p/C_V (dimensionless)

r_{cp} = critical pressure ratio (dimensionless)

In the aerodynamic model, the ratio of the desired flow velocity to the Mach number, F_{RM}, is selected as an input. Attainment of this velocity depends on the ratio r_n of the nozzle height, h_{noz}, to the irradiation zone or beam height, h_{iz}, for the diverging section of the supersonic nozzle. For isentropic expansion conditions the following relation is used to calculate this dimensionless ratio:

$$r_n = \frac{1}{\sqrt{[1/F_{RM}^2][A((\gamma+1)/(\gamma-1))]}} \tag{40}$$

where:

$$A = \left[\frac{2}{(\gamma+1)}\right]\left[1 + \left(\frac{\gamma-1}{2}\right)(F_{RM}^2)\right] . \tag{41}$$

With the height ratio, one can solve numerically for the ratio, r_p, of the pressure of the syngas in the irradiation zone, P_{iz}, to that in the plenum upstream of the nozzle throat. Newton's method can be used to solve for r_p from the following equation, also for isentropic flow:

$$\frac{P_{iz}}{P_o} = r_n = \frac{1}{\left(\sqrt{(\gamma-1)/2}\ (2/(\gamma+1))^{[1/2(\gamma+1)/(\gamma-1)]}\right)} \cdot$$

$$\sqrt{(1-r_p^{[(\gamma-1)/\gamma]})} \cdot r_p^{(1/\gamma)} \qquad (42)$$

In order to obtain the desired temperature, T_{iz}, in the irradiation zone, the upstream plenum temperature must be higher to allow for expansion cooling. The plenum temperature, T_o, is calculated as follows:

$$T_o = T_{iz}/r_p^{[(\gamma-1)/\gamma]} . \qquad (43)$$

Now that the nozzle pressure, temperature, and height requirements have been calculated as a function of the desired reaction zone conditions, the nozzle length is chosen to obtain sufficient nozzle throat area to handle the syngas volumetric flow. The volumetric flow V_{syn} is easily calculated from the feedrate via the perfect gas law. The nozzle length, L, is identical to the irradiation zone length and is utilized in the photolysis calculations. It is calculated from the volumetric flow and nozzle height as follows:

$$L = \frac{V_{syn}}{v h_{noz}} \qquad (44)$$

where:

L = the nozzle length (cm)

V_{syn} = the volumetric flowrate (cm^3/sec)

v = the syngas velocity in the irradiation zone (cm/sec)

h_{noz} = the nozzle height (cm).

Since the syngas is available from the gasifier at a very high pressure, considerable pressure reduction is required prior to entering

the nozzle plenum. A gas expansion turbine can be used to reduce pressure and at the same time recover energy. Downstream of the nozzle and collector the syngas will require recompression. The design and interfacing of the required turbine, compressor, and power recovery scheme will be considered in a later subsection on process energy requirements. The sulfur collector and laser design requirements will be considered first.

Modeling and design of the sulfur collector. Energy recovery considerations would make it desirable to collect HS fragments at a pressure higher than that in the irradiation zone. If this were the case, an aerodynamic converging/diverging nozzle could be used to recover part of the pressure drop loss in going from the higher initial pressure in the plenum to the lower pressure required in the irradiation zone. On the other hand, collisional kinetic considerations make it desirable to collect at a pressure less than that in the irradiation zone. The upper pressure limit in the irradiation zone is, in fact, determined more by the downstream collection pressure than by the laser beam attenuation by photon absorption at higher densities. Although it is necessary to collect the HS photofragments relatively close to the irradiation zone, i.e., before they have a chance to recombine with each other, having a collector apparatus in the flow stream prevents efficient pressure recovery such as could be obtained with a converging/diverging nozzle system.

Collector design is based on a simple collision theory as described below. If the mean free paths of an HS fragment, based on HS-HS collision rather than HS-CO or HS-H_2 collision, is less than the distance to

a collector surface, recombination is likely. The mean free path for HS collisions is given by:

$$\ell_{HS} = 1/(\pi\sqrt{2}\,\sigma_{HS}^2\,\rho_{H_2S}\,\theta_{ph}) \quad (45)$$

where:

ℓ_{HS} = the mean free path (cm)

σ_{HS} = the collisional cross section for HS-HS collisions (for typical diatomic species this is 3.5×10^{-8} cm^2)

ρ_{H_2S} = the H_2S number density (calculated from the H_2S partial pressure)

θ_{ave} = the average photolytic cut.

It is also useful to calculate the molecular speed (in a random direction) of an HS fragment, v_{HS}, and the average time between HS-HS collisions, t_{coll},

$$v_{HS} = \frac{8\,RT_{iz}}{\pi\,M_{HS}} \quad (46)$$

and

$$t_{coll} = \frac{1}{\sqrt{2}\,\pi\,\sigma_{HS}^2\,v_{HS}\,\rho_{H_2S}\,\theta_{ave}\,m_{coll}} \quad (47)$$

where:

v_{HS} = HS fragment speed (cm/sec)

R = gas constant = 8.314×10^7 erg/g-mole (K)

T_{iz} = gas temperature in irradiation zone (K)

M_{HS} = molecular weight of HS (33 g/g-mole)

m_{coll} = ratio of the collector pressure to the irradiation zone pressure

t_{coll} = time between HS-HS collision (sec) and

σ_{HS}, ρ_{H_2S}, θ_{ave} are as defined previously.

The reported rate of the recombination reaction can be used to calculate the recombination reaction half-life using a solution to the differential equation for second order reaction kinetics:

$$t_{1/2} = 1/(k \cdot \rho_{H_2S}\ \theta_{ave}\ m_{coll}) \qquad (48)$$

where:

k = the reaction rate constant (sec^{-1}).

For the rate constant reported in the literature of 3×10^{11} the resulting baseline half-life of 2.5×10^{-4} sec is greater than the average time between HS-HS collisions of 3.3×10^{-5} sec. These data indicate that HS fragments can be collected in a time period much shorter than the half-life for the recombination reaction. Accordingly the recombination yield, X_{rec}, can be low and the post-photolysis yield, θ_{pp}, can be high.

Figure I.7 in the previous subsection shows the fraction of dissociated H_2S, or HS fraction, captured by a given collector as a function of H_2S pressure and was calculated from the equations below. At very low pressures, few collisions take place before a large fraction of the HS fragments are collected. At higher pressures, a large fraction of the HS fragments collide, hence a recombination reaction takes place before collection is possible and the theoretical dissociated HS fraction falls to 0.5, the equilibrium value from Equation (35). A post-photolysis yield of 0.5 in a commercial process implies that the process could only remove half the sulfur during each pass by the laser beam. A recycle arrangement or a system incorporating multiple passes of gas through the laser beam would be required. Process complexity considerations make a single pass system with both photolytic, θ_{ave}, and HS-fragment removal cuts θ_{pp} of 0.99+ highly desirable.

From Figure I.7 it is seen that θ_{pp} decreases with increasing HS partial pressure, and by Equation (47) θ_{pp} also decreases as the time between HS fragment collisions decreases. The shapes of the curves in the figure suggest an exponential relationship as follows:

$$\theta_{red} = e^{-K/t_{coll}} \tag{49}$$

where:

θ_{red} is a reduced HS fragment removal yield = $(\theta_{pp} - 0.5)/0.5$ (50)

K is a constant

t_{coll} is the average time between HS-HS collision.

Since the reaction half-life, $t_{1/2}$, varies inversely with pressure [Equation (48)] in the same manner as t_{coll} [Equation (47)], a new dimensionless exponent for Equation (49) is suggested. This new exponent, a, is the ratio of the time an HS fragment has to travel to a collector surface, t_{surf}, to the time at which one-half of the HS fragments will have reacted with each other, $t_{1/2}$. Thus Equation (48) becomes

$$\theta_{red} = e^{-(t_{surf}/t_{1/2})} = e^{-a} . \tag{51}$$

As the ratio a increases, the recombination reaction becomes increasingly dominant. For the design problem a total cut, θ_{tot}, value of 0.98 is needed. It can be shown that this occurs when (a) is considerably less than unity, i.e., the HS fragment must with high probabelity strike the collector surface before encountering another HS fragment. Equation (51) can be solved for t_{surf}. Since the velocity of an HS fragment is known from Equation (46), the shortest distance an HS fragment can travel to assure 99+% collection is calculated as follows:

$$d_{tube} = \frac{v_{HS}}{t_{surf}}$$

where:

v_{HS} = the HS fragment speed (cm/sec) calculated from Equation (46)

d_{tube} = minimum travel distance for HS fragment (cm)

t_{surf} = travel time in seconds from Equation (51).

The small minimum distance, d_{tube}, can serve as a design criterion for a variety of possible collector designs. It could represent a minimum mesh size for a screen-type collector or a minimum tube size for a multipore or "honeycomb" collector system. Figure I.10 illustrates four such concepts. A continuously moving or periodically removed collector would be necessary to prevent plugging of the pores with sulfur or metallic sulfur compounds.

The experiments of Chen and Borzileri[118] performed at syngas pressures of 300 to 600 torr showed HS fragment collection yields in the range 0.5 to 0.8 at H_2S partial pressures around 2 millitorr as shown in Figure I.11 which includes data from their report. Their collector, however, was quite large, with tubing diameters of 15 and 30 cm. For such large distances for HS fragments to travel, the probability of recombination is high, as verified by their results. Their results also indicate a dependence of the collection yield on the syngas total pressure rather than just the HS partial pressure. With the large diameter collector, the collisional dynamics of the HS-CO and HS-H_2 system has a greater effect on the process and a different model would be required. For this sub-centimeter collector and the fewer collisions

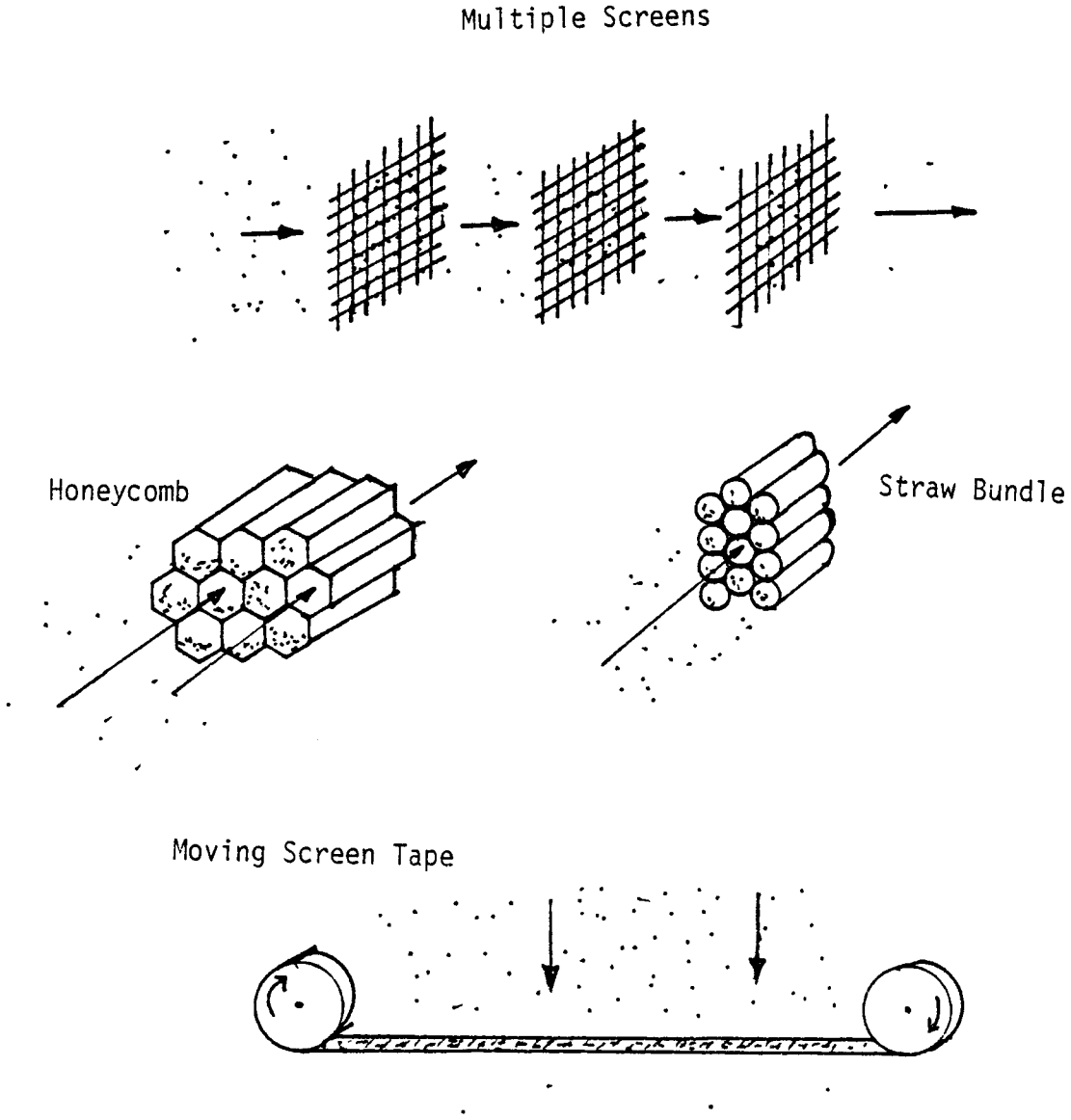


Figure I.10

Collector Concepts

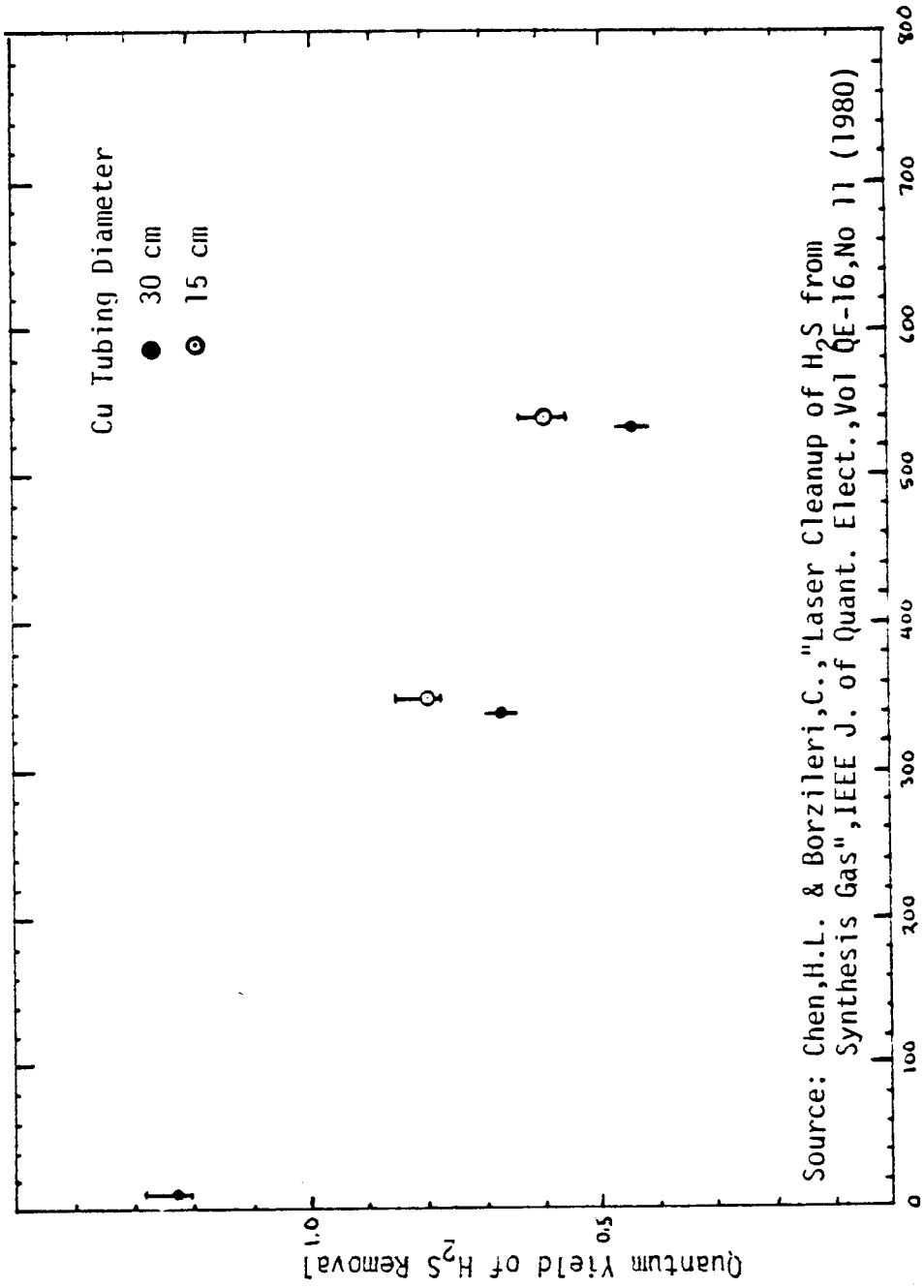


Figure I.11

Quantum Yield of H_2S Removal at Various Synthesis Gas Pressures

encountered, the HS-HS collisions model should prove adequate for design scoping purposes.

The laser system design model. In the subsection above, the fluence or energy per unit area of reaction zone cross section required for photodissociation was calculated. The device which delivers this energy, the laser, is best thought of as an energy conversion device which converts electrical and/or chemical energy into coherent, intense radiation. Two basic modes of energy output are available, depending on the type and design of laser utilized. A continuous wave (CW) laser emits a continuous stream of photons at a constant power per unit of beam cross sectional area. The more common pulsed laser emits its photon energy in very intense pulses, generally of very short duration, i.e., on the order of 10^{-7} sec, at a predetermined pulse repetition rate (PRF) or pulse frequency. Assuming the use of a frequency-shifted ArF laser operating in the ultraviolet at a wavelength of 210 nanometers, the problem of sizing the laser to the task described above must be treated. A short description of such a laser, however, is useful beforehand.

The ArF laser falls in a class of chemical lasers known as rare-gas halide (RGH) lasers. The output energy is a result of the lasing of the ArF eximer, during which the unstable rare-gas compound dissociates. Electric energy is used to excite the argon and fluorine to levels at which the ephemeral eximer can exist. A gas flow loop allows regeneration and reuse of the Ar and F_2 reactants. An ArF laser by itself produces a UV frequency of 193 nm. Introduction of a scattering medium, such as hydrogen, allows a spectroscopic Stokes shifting of the

frequency to a lower energy. The physics of the Stokes shift will not be discussed; however, the photodissociation frequency of 210 nm is created in this manner.

The laser pulse energy requirement is calculated from the fluence and the cross sectional area of the beam required by the irradiation zone dimension.

$$E_p = \phi_{fo} A_{beam}$$

where:

ϕ_{fo} = initial beam energy fluence (joules/cm^2)

A_{beam} = beam cross sectional area (cm^2) = $h_{iz} \cdot V_{beam}$

E_p = laser energy per pulse (joules/pulse).

The syngas flow past the laser beam is continuous, hence the pulse rate or PRF must be set such that every slug of gas passing through the irradiation zone is struck by the laser beam. The transit time of a slug of gas through the beam is calculated as follows:

$$t_b = \frac{W_{beam}}{v_{gas}} = \frac{W_{beam}}{M\ v_s}$$

where:

t_b = the transit time (sec)

W_{beam} = the laser beam width in the gas flow direction (cm)

M = the Mach number of the gas in the reaction zone

V_g = the velocity of the syngas through the reaction zone

v_s = the sonic velocity of the syngas (cm/sec).

The required PRF in Hertz is the reciprocal of the transit time:

$$PRF_{req} = 1/t_b \ .$$

At high gas speeds and with small laser beam cross-sectional dimensions, such as a 1 cm x 1 cm beam, the laser system PRF required is on the order of tens of thousands of pulses per second (10^4 Hz). Because of power supply limitations and the need for lasing zone recovery, single high-power RGH lasers of this type are usually limited in PRF to the range of 1000 to 1500 Hz. One possible way to live within this limitation is to increase the transit time by increasing the laser beam width. To do so, however, introduces optical and diffraction problems encountered with beams very oblong in cross-section, that is those with aspect ratios (W_{beam}/h_{iz}) greater than 2. The beam height is fixed by the nozzle flow and nozzle height requirements, hence the latitude in width adjustments is small. Another consideration is the fact that typical high power laser beams are available at full fluence over areas of only a few square centimeters. A technical solution to the high PRF requirement exists. By temporally multiplexing, i.e., time phasing, a number of laser sets to fire sequentially, a laser system can be designed with arbitrarily high system PRF. By this means, every slug of gas can be irradiated. The number of sequentially timed sets needed is calculated from the required system PRF and the maximum PRF available from a single laser unit or laser "head":

$$N_{set} = \left(\frac{PRF_{req}}{PRF_{max}}\right), \text{ rounded upward to the next integer.}$$

Given the PRF_L less than or equal to PRF_{max}, the laser output power in watts can be calculated as follows:

$$P_L = E_p \, PRF_L$$

where:

E_p = the pulse energy in joules/pulse

PRF_L = the laser repetition rate of the lasers in each timed set (Hz or sec^{-1})

P_L = the output power (watts).

The output power in watts is the most common term used to describe laser performance. A constraint is also introduced by this variable. In addition to PRF limitation, a power limitation per laser head can also exist; thus for a given power requirement per set of lasers, multiple heads may be required. The physics and geometry of the lasing cavity usually imposes such limits. For the laser system of interest here, a 1240 watt output head is considered a maximum. The number of heads per laser set can be calculated from the required set power and the maximum power per head:

$$N_{hd} = \left(\frac{P_s}{P_{max}}\right), \text{ rounded upward to nearest integer,}$$

where:

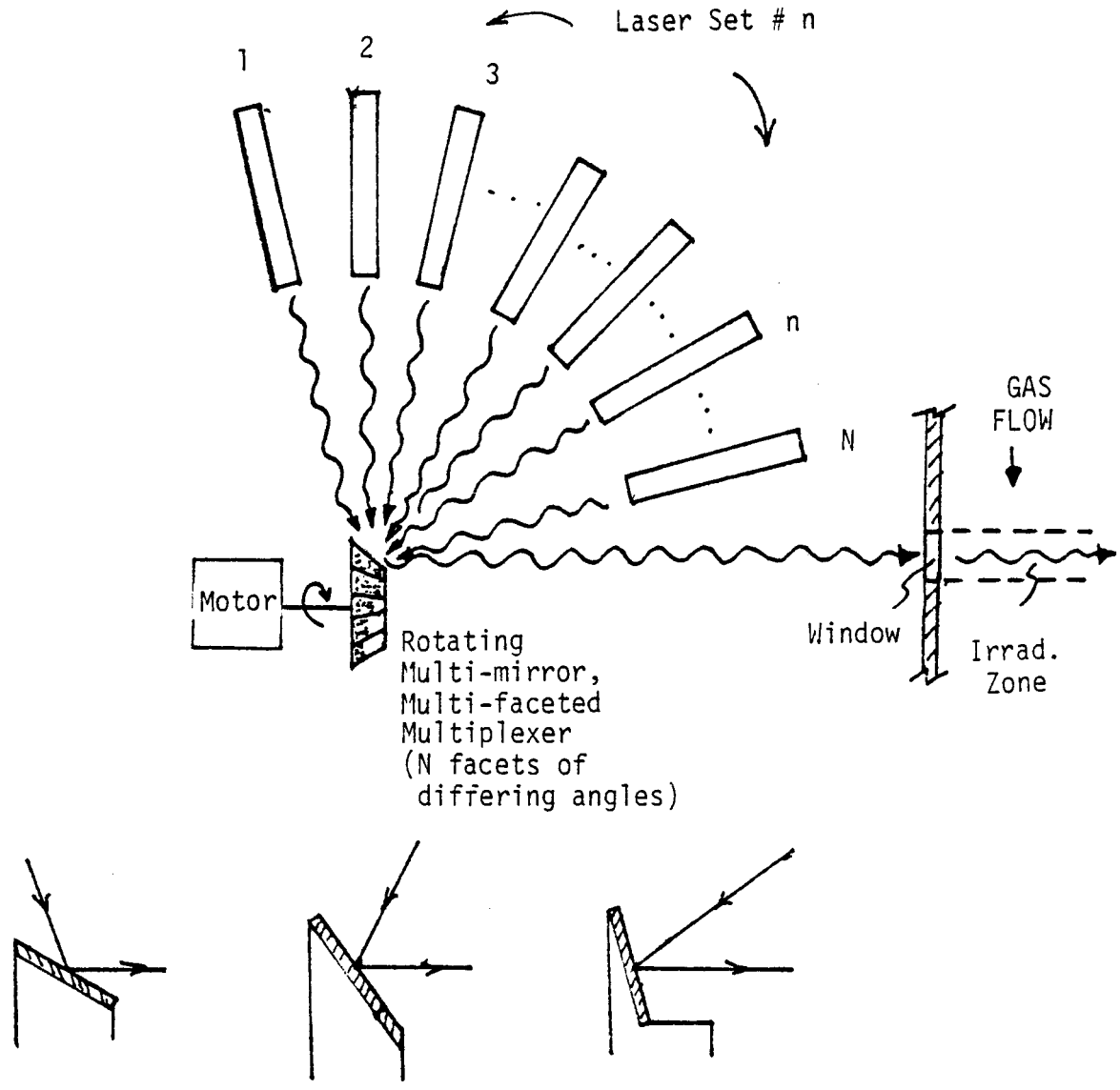
P_s = the output power requirement for one timed set of lasers (watts)

P_{max} = the maximum output power of a laser head

N_{hd} = the number of laser heads per set.

The total number of laser heads required for the process can be calculated from the product of the number of laser sets and the number of heads per set.

Arrangement and design of the laser optics, beam handling, and multiplexing equipment will not be discussed here. Figure I.12 shows a



Facet Corresponding to Laser Set # n

Figure I.12

Laser Beam Configuration

configuration by which multiple laser beams can be routed into the irradiation zone.

Only a small fraction of the energy input to a laser system is converted to coherent monochromatic (one-color) light. The remainder is dissipated as heat which must be removed. As with many other devices which convert energy from one form to another, the ratio of desired output energy, in this case laser light, to the energy input, in this case electrical power, is expressed as an efficiency. The laser efficiency is a frequently quoted hardware performance variable, and its improvement, is a goal of laser development efforts. The overall laser efficiency utilized in this example includes component efficiencies for such laser subsystem as the power supplies, gas circulation system, and the lasing medium. The design input power for the laser system is calculated as follows:

$$P_{in} = \frac{P_{L_{tot}}}{e_L \, F_p}$$

where:

P_{in} = the design input line power required for the laser system (watts)

$P_{L_{tot}}$ = the total laser output power requirement (watts)

e_L = the total laser power efficiency (dimensionless)

F_p = a power factor, usually between 0.9 and 0.99, to allow for some overdesign of the power supplies.

Laser efficiencies are quite low compared with energy conversion efficiencies familiar to chemical and mechanical engineers. Hence, if tens of kilowatts of photon power are required, the laser system can be

a significant contributor to plant energy requirements. In order to consider further the process energy calculation, the power requirements and output for the compressor and turbine will be discussed next.

Pre- and post-nozzle gas conditioning. Since the partially cleaned syngas from the coal gasifier and Rectisol units at 31 atmospheres must be reduced to the pressure in the nozzle plenum prior to photolysis, considerable mechanical work is available if turbines are used to reduce the pressure. Three turbines in series are used to obtain reasonable pressure drops across the blades of each and to allow reheating between each turbine. Reheating is necessary to prevent condensation of the synthesis gas inside the turbines. Generator sets can be connected to each turbine and it is assumed that the electric power generated can either be used elsewhere in the plant or sold to the supplying electric utility at the same price at which power is purchased. Part of the thermal energy for reheating the syngas between turbines is obtained from the heat of compression downstream of the collector via a heat exchange system.

The pressure ratio for each turbine is obtained from the total pressure ratio from plenum to gasifier and the number of turbines as follows:

$$P_t = \left(\frac{P_o}{P_{gas}}\right)^{1/n_t} ,$$

where,

P_o = the plenum pressure (atm),

P_{gas} = the gasifier pressure (31.6 atm), and

n_t = the number of turbines in series.

The work from each turbine is calculated from isentropic expansion relationships as follows:

$$W = \frac{m_o \, R \, T_{gas} \, (\gamma/(\gamma-1))[1-P_t^{((\gamma-1)/\gamma)}]}{525600(42.408)} ,$$

where:

W = work in horsepower,

m_o = molar flow rate of syngas (lb moles/min),

T_{gas} = temperature at turbine inlet (K),

R = gas constant ($1.98 \frac{BTU}{g \text{ mole-R}}$),

γ = heat capacity ratio (1.406),

P_t = pressure ratio in a turbine, and

Conversion factors = 525600 min/yr; 42.4 BTU/min/hp.

The absolute temperature at the outlet of each turbine is calculated as follows:

$$T_{to} = T_{coal} \, (P_t)^{(\gamma-1/\gamma)} ,$$

where T_{coal} is the absolute temperature of the entering high-pressure syngas and P_t and γ are defined above.

The inlet syngas to turbines 2 and 3 is assumed to be reheated to the same temperature at which it entered the first turbine g, i.e., 560 R or 100°F.

The recompression of the photolyzed syngas prior to methanol synthesis consumes a significant portion of the energy needed for this application. Fortunately, a petrochemical or synfuels complex will have available high-pressure, 600 psig, steam which can be used to drive compressors at a cost lower than that for electric motor driven

compressors. The decontaminated synthesis gas leaves the collection region at close to an atmosphere and must be recompressed to the reactor inlet pressure of 76 atmospheres and reheated to 448°F. Detailed compressor calculations performed with the assistance of D. W. Langenberg[119] indicate that four compressors in series are needed for the baseline task, with an additional compressor added if the collector operates below atmospheric. The design equation for compressors is very similar to the turbine design equation except that many terms are inverted and compressor efficiency terms must be added. For the baseline process, four compressors with differing suction volumes were designed and costed. Table I.2 shows these costs and volumetric flow rates. Should the syngas flow requirements vary, the following equation scales the suction volume:

$$V_s(i) = V_{sb}(i) \frac{F}{F_{(b)}} ,$$

where:

$V_s(i)$ = suction volume of the ith compressor,

$V_{sb}(i)$ = suction volume of the ith baseline compressor,

F = actual syngas flow rate (SCFM), and

F_b = baseline syngas flow rate (SCFM).

If the collector pressure is above atmospheric, the suction volume of the first compressor can be reduced by the ratio of inlet pressures:

$$V_s(1) = \left(\frac{1}{P_{coll}}\right) V_{sb}(1) ,$$

where P_{coll} is the collector pressure (atm).

Table I.2

Baseline Compressor Design Data

Compressor No.	Suction Volume (cfm)	Output Temperature (°F)	Required Cooling (Btu/yr)	Power (HP)	Cost ($MM)
	0.0	31.0.	0.00E+00	0.0	0
1	79865.4	277.0	0.20E+12	8994.8	2098154
2	28052.7	295.0	0.22E+12	9593.8	1249045
3	9384.2	295.0	0.22E+12	9593.8	799501
4	3494.1	299.0	0.22E+12	9753.6	560645

During each compression step, the syngas undergoes considerable heating. The heat of compression must be removed by heat exchangers and can be used to reheat the syngas exiting the turbines. Since the methanol production reactor requires hot gas, the last compression stream is not cooled. It requires additional heat from the 600 psig steam to reach the 448°F required for methanol synthesis. Since the coolant temperature required for compressor intercooling is less than that of the fluids returning from the turbine reheating, a chiller must be installed. An energy management system to recover as much thermal energy as possible was designed for the overall gas handling system and is shown schematically in Figure I.13. Scaling equations for the heat exchanger loads are included in the process model to calculate off-baseline requirements, but are not discussed here.

Process building layout. The building to house the photolysis facility building must be sized adequately to house the nozzle, collector, turbines, compressors, and laser system. The floor areas for each system scale in some manner with the capacity or size of the equipment. Most of the factors used are scaled to the baseline design using the following generic relationship:

$$A_{new} = A_{base} \left(\frac{Q_{new}}{Q_{base}}\right)^{n},$$

where Q is an equipment attribute and n is a scaling exponent.

Figure I.14 shows the layout of the baseline syngas removal facility. The following eight relationships calculate the areas for off-baseline design process conditions. The variable names in the actual

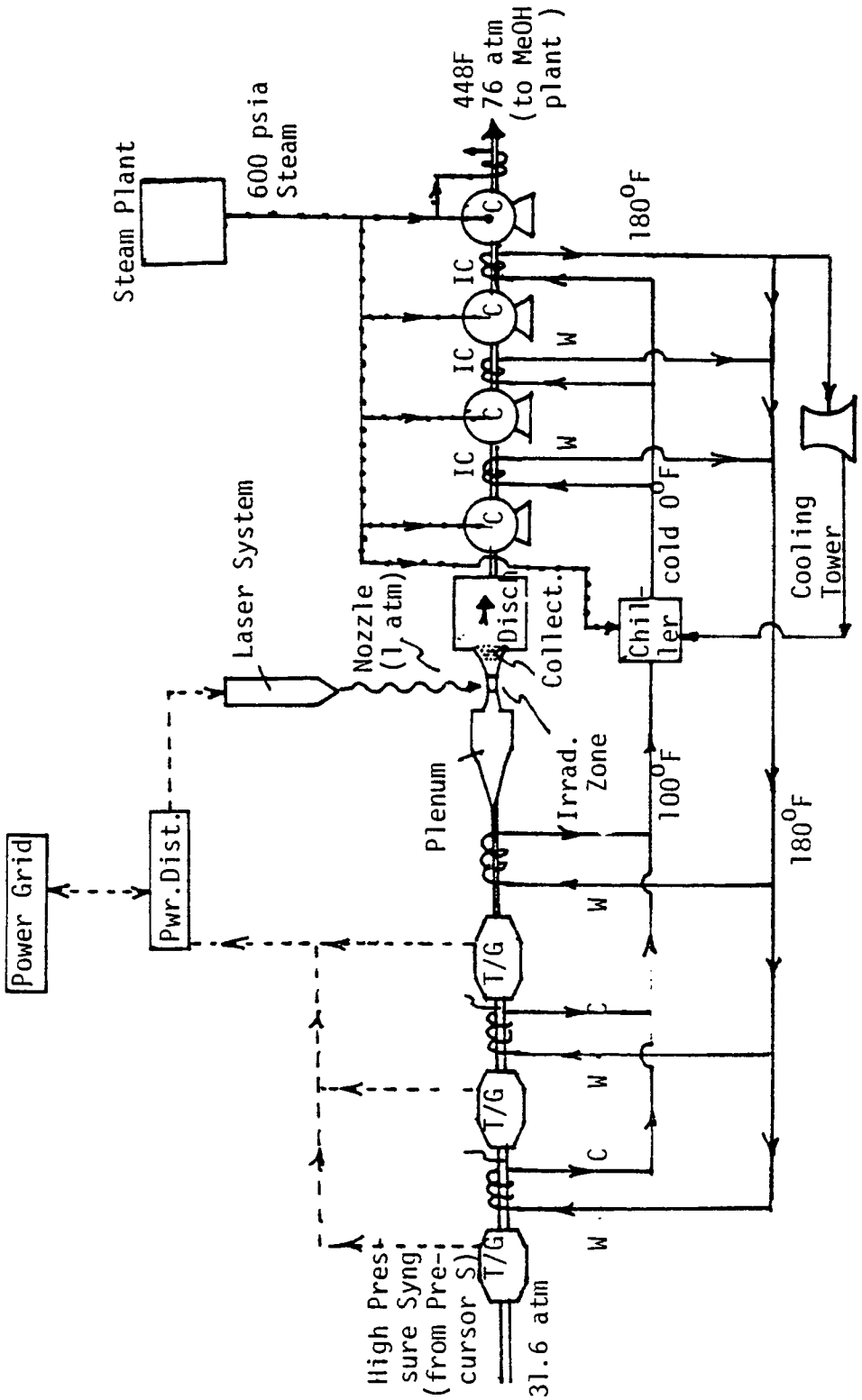


Figure I.13

Schematic of Energy Management System

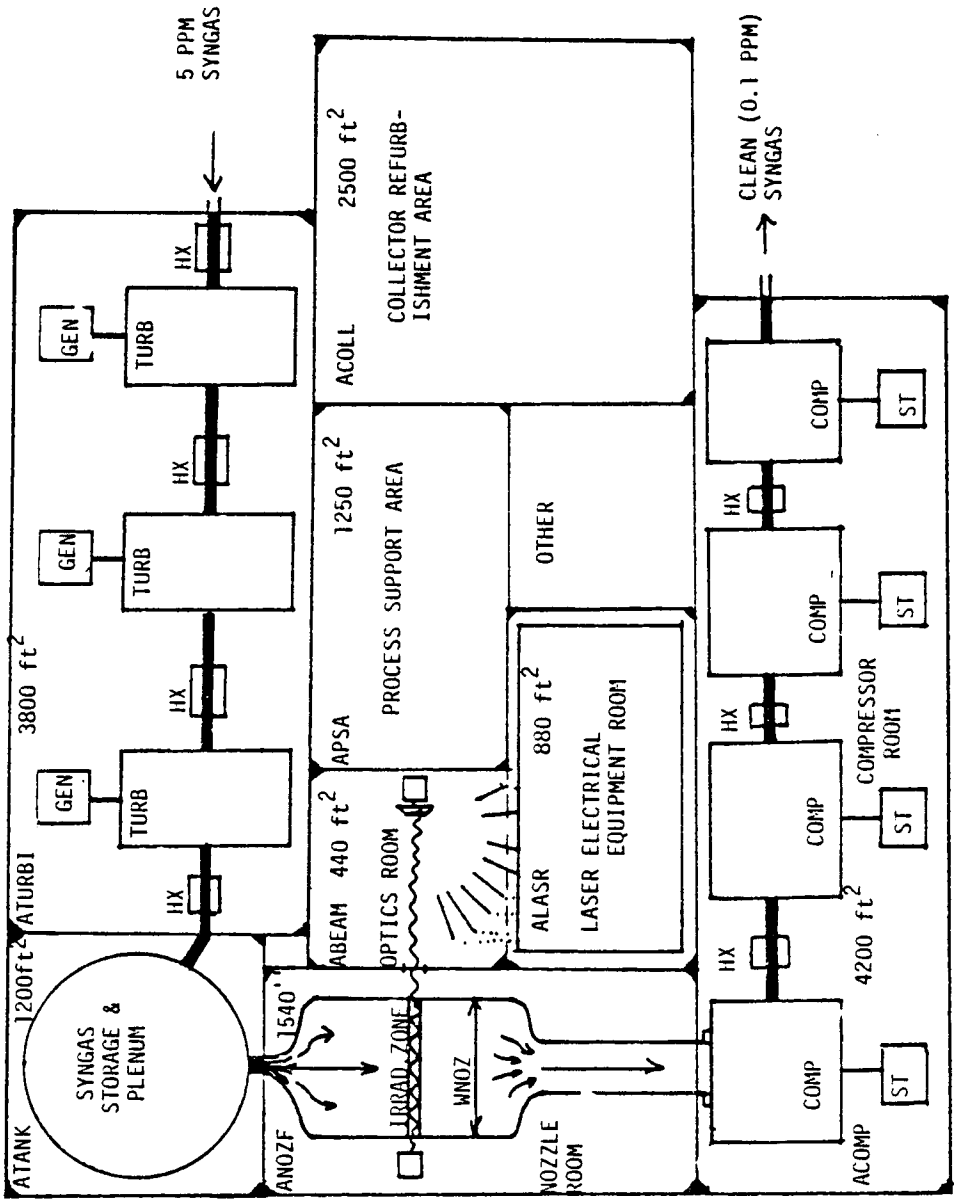


Figure I.14

Baseline Facility Layout

FORTRAN layout routine in Appendix J are used. Baseline values for the various areas are indicated in parentheses.

1. Nozzle and photolysis reactor:

$$ANOZF = 50. * (WNOZ/30.48 + 5.)$$

where WNOZ is the irradiation zone length in cm (788 cm in baseline) and ANOZF is the required floor area in ft^2 (~1540 ft^2 in baseline).

Essentially the equation states that the nozzle floor area is 50 ft times the irradiation zone length in feet, with 5 extra feet allowed for access.

2. Turbine and generator area:

$$ATURBI = 40. * 95. * (WTURB/WTURBB) ** 0.6 ,$$

where:

WTURBB = the total baseline work production of all three turbines (hp), (16970 hp),

WTURB = the off-baseline work produced (hp), and

ATURBI = the floor area required.

In the baseline a 40 x 95 ft area (3800 ft^2) was allowed for the three turbines and generators. Since the work terms include both throughput of gas and pressure drop in their calculation, the turbine horsepower production was deemed an appropriate scaling variable.

3. Compressor floor area:

$$ACOMPR = 35. * 120. * (WCOMP/WCOMPB) ** 0.6 ,$$

where:

WCOMPB = the total baseline power requirement for four compressors (37936 hp),

WCOMP = the off-baseline power requirement (hp), and

ACOMP = the total floor area for compressors.

For the same reasons as for the turbine category above, power was chosen as the scaling variable.

4. & 5. Laser and beam handing area:

$$ALASR = 40. * NHEAD * (POWHD/POWHDB) * 0.5$$

$$ABEAM = 20. * NHEAD ,$$

where:

NHEAD = the number of laser heads required for photolysis,

POWHD = the power output of each head (watts),

POWHDB = the power output of a baseline design laser head (1238 watts),

ALASR = the floor area required for the laser heads and associated structural support hardware, and

ABEAM = the floor area required for optical and beam handling equipment, including optical benches.

Since multiple laser heads are needed for supplying the photolysis energy, enough area must be provided for the support racks and power supplies needed for each. A single 1238-watt baseline laser head and its associated equipment is allowed 40 ft^2 of space. A power scaling term is included to allow for variation of the laser head size with differing power requirements. The space required for optical and beam handling equipment depends on the number of laser heads which must be serviced by these arrays of optical elements.

6. Collector refurbishment area:

$$ACOLL = 2500. * (MOSULF/MOSULB) ,$$

where:

MOSULF = the amount of sulfur removed by the collector per year (g-moles/yr),

MOSULB = the amount of sulfur removed in the baseline design (297500 g-moles/yr), and

ACOLL = the area required for the refurbishment, i.e., their cleaning and refabrication (ft^2), of process collectors.

The baseline facility is designed with a floor space of 2500 ft^2.

7. Syngas storage tank floor space:

$$ATANK = 1200. * (MOFLOW/MOFLWB) ** 0.666 ,$$

where:

MOFLOW = the syngas flow rate to the nozzle (lb-moles/yr),

MOFLWB = the baseline syngas flow rate to the nozzle (1.3375×10^8 lb-moles/yr), and

ATANK = the floor area required for a spherical holdup tank for incoming syngas (ft^2).

The baseline 30-ft-diameter spherical tank requires 1200 ft^2 of floor area.

8. Process support areas:

$$APSA = 1250. * (MOFLOW/MOFLWB) ,$$

where:

MOFLOW and MOFLWB are defined above, and

APSA = the floor area required for support functions (ft^2).

The floor area required for process support functions such as maintenance and operation is assumed to scale with the amount of syngas handled.

Total area:

$$ATOT = ANOZF + ATURBI + ACOMPR + ALASR + ABEAM + ACOLL + ATANK + APSA .$$

The total floor is calculated as the sum of the above areas. The building here depicted would most likely be an add-on to another larger building. This total area, ATOT, is to be used for estimating the cost of this add-on facility.

Development of Cost Models

Construction of the Economic Model

The two major models illustrated here are the capital and operating cost scaling models. A simple RAM model is also included to illustrate a simple method of handling first-order component lifetime implications.

The capital cost scaling model. Over twenty direct capital cost centers have been identified for cost scaling in this example. Rather than describe each equation separately, Tables I.3 and I.4 present both the cost scaling equations and an input glossary. The source of an input and its baseline value are included as a point of reference.

Basically, two types of equations are used. The first type simply multiplies the installed unit cost of a required component by the design requirement for that component or attribute. The second type represents a true scaling relation derived from a plot of installed equipment cost

Table I.3

Capital Cost Scaling Relations

1. Nozzle, plenum, collector, and photolysis chamber:

   CNOZ† = 200 * WNOZ†† ($200/cm)

2. Spare collector units:

   CLSPR = CLUNIT * 10 (10 units required)

   where CLUNIT = 168.8/TUBED (Collector cost is inversely proportional to pore diameter)

3. Laser system cost (including heads and power supplies):

   CLASR = CCPWAT * WATTAV

4. Beam transport system cost:

   CBEAM = 0.2 * CLASR (0.2 ≡ 20% of category 3 above)

5. Optical multiplexer cost:

   CMPXR = 10000 * (NHEAD/NHEADB)

6. Spare optical units

   COSPR = COUNIT * 5 (5 units required)

7. Turbines (total for 3)

   CTURB = [E1 * 48 * (WTURB/3) ** 0.93] * 3

8. Generators (connected to turbines, total for 3)

   CGEN = [E1 * 30 * (WTURB/3) ** 0.93] * 3

9. Turbine reheaters (total for 3)

   CHEXT = (E1 * 70.8 * ATURB ** 0.83) * 3

†All costs in 1982 $
††Table I.4 describes the input variables

Table I.3 (Continued)

10. Compressors

$$CCOMP = \sum_{1}^{NCOMP} 10^6 * \{[SVOLN(I)/10000] ** 0.5\} * 0.707$$

11. Steam driven compressor turbines/motors:

$$CMOTC = E1 * NCOMP * 48 * (HPNT/NCOMP) ** 0.93$$

12. Compressor intercoolers:

$$CCUL = E1 * (NCOMP - 1) * 70.8 * [ACOMP/(NCOMP - 1)] ** 0.83$$

13. Chiller for compressor coolant:

$$CREFR = E1 * 1717 * TONS ** 0.665$$

14. Post compression reheat exchanger:

$$CMEX = E1 * 70.8 * AMEX ** 0.83$$

15. Piping cost:

$$CPIPE = E1 * 4 * SCFM ** 0.7$$

16. Syngas storage tank cost:

$$CTANK = E1 * 15.27 * SCALE ** 0.95$$

where:

SCALE = (DIA ** 2) * SQRT (PP), and

PP = (PO/760) * 14.7

DIA = 1.24 * (VOL ** 0.33)

VOL = 2 * SCFM * (760/PO)

17. Pumps for thermal energy management system

$$CPUMPS = E1 * 0.32 * QH$$

where QH = GPM * HEAD

Table I.3 (Concluded)

18. Instrumentation and control:

$$CIC = 1.E5 * (NHEAD/NHEADB)$$

19. Flow system preoperational checkout:

$$CPCHK = 76.E3 + 50 * WNOZ$$

20. Cooling water system for lasers:

$$CCW = 2.E5 * (WALLPG/3.64E6) ** 0.7$$

21. Outside utilities:

$$COUTS = 0.001 * POWRI + 0.001 * SREQ$$

22. Special shops:

$$CSS = 50000 * (MOSULF/MOSULB)$$

23. Electrical distribution system:

$$CEDS = 40000 * (KWCAP/KWCAPB)$$

24. Building cost:

$$CBLDG = 120 * ATOT \quad (\$120/ft^2)$$

Table I.4

Driver Inputs for Capital Cost Scaling Relations

Variable Name	Description	Units	Capital Cost Equation Number	Source	Baseline Value
WNOZ	Irradation zone length	cm	1	Performance code (photolysis)	788.2 cm
CLUNIT	Unit cost of a collector	$/unit	2	Economics code (collector)	$800
TUBED	Collector pore diameter	cm	2	Design code (collector)	0.211 cm
CCPWAT	Cost per watt of laser output	$/W	3	Cost input data	$500
WATTAV	Required laser power for photolysis	watts	3	Performance code (photolysis)	27100 watts
NHEAD	Total number of laser heads		5	Design code (laser system)	22
COUNIT	Unit cost of irradiation zone boundary optics	$/unit	6	Cost input data	$800
WTURB	Total expansion work from all 3 turbines	hp	7,8	Design code (turbines)	16970 hp
E1	Cost Escalation factor (FY 1978 to FY 1982)		7-16	Input data	1.46
ATURB	Heat exchanger tube area for each turbine	ft^2	9	Design code	685 ft^2

Table I.4 (Continued)

Variable Name	Description	Units	Capital Cost Equation Number	Source	Baseline Value
SVOLN(I)	Compressor suction volumes	ft^3/min	10	Design code (compressors)	79865 cfm 28053 9384 3494
NCOMP	Number of compressors in series		10-12	Design code	4
HPNT	Total compressor power	hp	11	Design code (compressors)	37940 hp
ACOMP	Total tube area for compressor intercoolers	ft^2	12	Design code (energy management)	2966 ft^2
TONS	Refrigeration load for compressor coolant	tons	13	Design code (energy management)	2966 ft^2
AMEX	Heat exchanger tube area for post-compression reheat	ft^2	14	Design code (energy management)	128 ft^2
SCFM	Syngas volumetric flow	scfm	15,16	Performance code (material balance)	91360 scfm
PO	Plenum pressure	torr	16	Design code (aerodynamics)	1442 torr
GPM	Coolant pumping requirements	gpm	17	Design code (energy management)	4710 gpm

Table I.4 (Continued)

Variable Name	Description	Units	Capital Cost Equation Number	Source	Baseline Value
HEAD	Pumping head for coolant pumps	ft of H_2O	17	Design input	40 ft.
WALLPG	Line input power to laser system	watts	20	Design code (laser system)	2.71×10^6 watts
POWRI	Total installed electric power requirements	MW	21	Electric power code	6.85 MW
SREQ	Steam requirements for compression and reheat	lb/yr	21	Design code (energy management)	2.18×10^9 lb/yr
MOSULF	Gram mols of S removed per year	g mols S/yr	22	Design code (material balance)	2.97×10^5 g mols/yr
MOSULB	Baseline gram mols of S removed per year	g mols S/yr	22	Baseline design	2.97×10^5 g mols/yr
KWCAP	Total installed electrical capacity	kW	23	Electric power code	6852
KWCAPB	Baseline design electrical	kW	23	Baseline design	6852
ATOT	Total add-on building area	ft^2	24	Capital cost code (layout)	15813 ft^2

versus capacity such as found in cost estimating manuals and in numerous articles such as that by Diaz and Pikulik.[120] Usually presented as log-log plots, these relations are easily translatable to equations of the form $C = kA^n$ by evaluating the slope in the range of interest. Since many of the relations used were expressed in 1978 dollars, an escalation factor (E1) of 1.46 has been used to translate the cost to 1982 dollars.

The summation of the above costs for each cost center, CCTOT, constitutes the facility direct costs. The indirect costs, i.e., engineering, contingency, and interest during construction, are handled as described below.

Since no actual engineering design and cost estimate was prepared for this project, the assignment of an engineering and contingency to each individual cost center was impossible. By considering the composite allowances utilized for other proposed energy projects in the photochemistry field, however, a reasonable value can be derived.

Engineering: Since in this instance a significant portion of the equipment is high technology and the remainder conventional, one can conclude that the engineering allowance should exceed values typical of conventional technology, the latter typically on the order of 10 to 15 percent of direct costs. Since the laser system is the largest capital cost, hence carries considerable weight, an overall engineering allowance of 25% for the entire process was considered appropriate,

$$CENG = 0.25 * CCTOT .$$

The new capital cost subtotal is now calculated,

$$C1TOT = CCTOT + CENG .$$

Contingency: Contingency allowances should be separately estimated for each detailed cost center. Since no actual engineering estimate was performed, contingency factors had to be assigned for aggregations of cost centers. Clearly the magnitude of the contingency depends on the detail level of the design, the complexity of the process, and the amount of experience the firm has had with the process. For laser-related equipment, for which little cost estimating experience is available, a 50 percent contingency is appropriate. Since the gas-handling and balance-of-plant equipment is a novel arrangement of conventional equipment, a contingency allowance of 30 percent is used. The project contingency is calculated as follows, using the costs generated according to the equations in Table I.3.

Laser equipment:

$$CONL = 0.5 * (CLASR + CBEAM + CCW + CIC + CMPXR + COSPR) .$$

Gas handling equipment:

$$CONGH = 0.3 * (CNO2 + CTURB + CGEN + CHEXT + CCOMP + CCCUL + CMEX + CTANK + CPIPE + CSS + CLSPR) .$$

Balance of plant:

$$CONBP = 0.3 * (CMOTC + CREFR + CPUMPS + CPCHK + COUTS + CEDS + CBLDG + CENG) .$$

The total contingency amount is:

$$CONTOT = CONL + CONGH + CONBP .$$

A composite contingency factor or fraction can be calculated as:

$$FCONAV = CONTOT/C1TOT .$$

For the baseline case the composite contingency is 41.3 percent.

The new subtotal is now calculated as:

$$C2TOT = C1TOT + CONTOT .$$

Interest during construction: Since this particular application involves a relatively small add-on facility to an existing plant, the construction time will be comparatively short. It is assumed that the UV lasers have been developed and can be fabricated in a relatively short time. Other large process items, such as compressors and turbines, are considered standard items which are deliverable in a few months from time of ordering. With these, perhaps optimistic, assumptions in mind, a construction time of one year has been assumed with nearly all construction money spent at the beginning of construction. For this reason the assumed interest rate of 10 percent also becomes the interest during construction (IDC). The IDC is taken as a fraction of the above subtotal, C2TOT:

$$CIDC = 0.1 * C2TOT .$$

The total capital cost is now calculated as:

$$CTOT = CIDC + C2TOT .$$

The baseline productivity, design, and associated capital costs will be presented after discussion of the operating cost scaling relations.

The operating cost scaling model. The operating costs consist of four parts: staffing, materials, utilities, and interest on working capital and inventories. Each will be considered in turn.

1. Staffing: Since the facility described here is an add-on facility, the staffing will be incremental. The fact that most of the process steps are continuous and that the physical size of this facility is small indicates a relatively small staff. In fact, all five commonly used categories, i.e., administration, operations, maintenance, component refurbishment, and support activities, need not be staffed.

Administration: One supervisory person with technical knowledge of the facility is assumed available for each of the five shifts. This person also acts as the facility operator. The following equation can be used for this category:

$$NSUPER = NSHIFT = 5 .$$

Operations: This role is filled by the supervisor above, and no other persons are required for this category, hence NOPER = 0 for all cases.

Maintenance: Since laser maintenance is assumed to be handled by an outside organization, a full-time maintenance mechanic is not needed for this facility, hence NMAINT = 0.

Component refurbishment: There are two components which fail on a regular basis and require continuing replacement. The irradiation zone optics are degraded by the high fluence of the laser beam, and for the base case must be replaced every 57 hours. In the later RAM discussions it will be seen that this lifetime, OPTLIF, is a function of fluence and is recalculated for each off-baseline case. To calculate the refurbishment labor, the number of optical units requiring replacement each year must be calculated:

$$OPRATE = (8760/OPTLIF) * AVAIL ,$$

where:

OPRATE = the number of units per year replaced

OPTLIF = the average optical unit lifetime (hrs),

AVAIL = the plant availability (calculated in the RAM model), and

8760 = the number of hours in a year.

It is assumed from an operations analysis study that one person, working one shift, can repair and replace 50 optical units per year. The number of optical unit refabricators is now calculated as

$$\text{NOPMAN} = \text{OPRATE}/50 \ .$$

Similar calculations can be made for the collector refurbishers who remove, clean, and reassemble the sulfur collectors. A typical collector lasts several hours and its lifetime COLLIF in hours defines the number which must be replaced per year.

$$\text{CLRATE} = (8760/\text{COLLIF}) * \text{AVAIL} \ .$$

If one person per shift can refurbish 100 per year, the work force requirement is calculated as

$$\text{NCLMNT} = \text{CLRATE}/100 \ .$$

It should be noted that these work force requirements are rounded upward to the nearest integer in the computer calculations.

Plant support: One clerical and technical support persons must be supplied on the day shift. For the baseline, one person in each category is assumed. If the plant capacity is increased significantly, the following scaling relation adds additional support staff:

$$\text{NSUPP2} = (\text{MOFLOW}/\text{MOFLWB})\ (1)$$

$$\text{NSUPP3} = (\text{MOFLOW}/\text{MOFLWB})\ (1) \ .$$

Total staff: The total staff is calculated from the sum of the above categories:

NSTAFF = NSUPER + NOPMAN + NCLMNT + NSUPP2 + NSUPP3 .

Salary categories: Calculation of labor costs requires multiplication of the staff size by the labor rates. Since each staffing category carries a different salary, the labor cost must be calculated for each category by itself and all categories summed. The annual wage rates were assumed for the various categories are shown in Table I.5.

Table I.5

Annual Wage Rates
for Staffing Categories

Category	Job	Class	Rate per year
Administrative	Supervisors	Monthly Salaried	$34,000
Component Refurbishment	Optics Refurbishment	Hourly	$20,000
	Collector Refurbishment	Hourly	$20,000
Plant Support	Clerical	Weekly Salaried	$14,000
	Technician	Weekly Salaried	$20,000

The subtotal labor cost is calculated as:

SALTOT = NSUPER * 34000 + (NOPMAN + NCLMNT) * 20000 +
NSUPP2 * 14000 + NSUPP3 * 20000 .

Fringe benefits: Fringe benefits are accounted for by adding 25 percent to the labor subtotal:

CSALT1 = 1.25 * SALTOT .

Contingency: A labor cost contingency of 20 percent is assumed for this first-of-a-kind process. The total labor cost is calculated as

$$\text{CLABOR} = 1.2 * \text{CSALT1} .$$

A summary staffing table for the base case labor calculation will appear in the later presentation of the baseline design.

Non-laser component replacement costs: The refurbishment operations described above require the purchase of repair or replacement components. The annual replacement rates were calculated above for the optical units (non-laser optics) and collectors and were lifetime dependent. The cost of replacement requires knowledge of the unit component costs, which constitute economic input data.

For the optical units:

$$\text{COPTIC} = 1.5 * (\text{OPRATE} * \text{COUNIT}) .$$

For the collectors:

$$\text{CRFURB} = 1.3 * (\text{CLRATE} * \text{CLUNIT}) ,$$

where COUNIT and CLUNIT are the costs of all replacement parts and supplies used in the rework of a single unit. The constants in front of each term in parentheses provide contingencies of 50% and 30%.

In addition to these major replaceables are work materials. Their annual cost is estimated to be 7% of annual labor costs and a 20% contingency is added.

$$\text{CAWM} = 0.07 * 1.2 * \text{CSALT1} .$$

The total cost for replacements is:

$$\text{CREPL} = \text{CAWM} + \text{CRFURB} + \text{COPTIC} .$$

Maintenance: A lump sum of $100,000 is assumed for maintenance items not included in the replacements category. If the plant capacity

is greatly increased, the following relation will increase this amount.

$$COPM = 1.E5 * (MOFLOW/MOFLWB) .$$

Total maintenance costs are calculated as:

$$CMAINT = COPM + COLP .$$

Laser operating costs: The laser is a special piece of process equipment for which maintenance, labor, and special materials are assumed to be purchased outside of the facility, hence, it is grouped under the materials category. Laser maintenance costs are often expressed in dollars per output watt-year as is the case here. Annual laser maintenance costs are calculated as follows:

$$COLP = OCPWAT * WATTAV ,$$

where:

OCPWAT = $/watt-yr of maintenance costs and

WATTAV = average laser output power (watts).

3. Plant utility costs: Calculation of major utility costs requires knowledge of the annual use of electric power, steam, cooling water, and compressed air. Various components of the utility requirements in each category are calculated in the design and equipment sizing portions of the overall model. A major category is that of electric power.

Electric power usage and cost: Power usage scaling equations are used to calculate the power use in kilowatts for several categories.

Laser:

$$KWLAS = WALLPG/1000 ,$$

where WALLPG = laser input power in watts.

Instrumentation and control: A lump sum of 100 kW is assumed.

$$KWIC = 100 .$$

Facility lighting:

$$KWLIO = 0.0017 * ATOT ,$$

where ATOT = the process add-on building area (ft^2).

Heating and ventilation:

$$KWHVO = 0.00823 * ATOT .$$

Recirculating cooling water pumps:

$$KWRCWO = 0.021 * (KWEQUI + KW) ,$$

where:

KWEQUI = the compressor intercooler heat load (converted to kW) and

KW = the reheat duty for turbine reheaters (converted to kW).

Coolant pumps for heat exchangers:

$$KWPUMP = 0.01 * GPM ,$$

where GPM = gallons per minute of coolant pumped.

Refrigeration power:

$$KWREFR = 0.725 * TONS ,$$

where TONS = the refrigeration load for the chiller.

The total power usage is calculated as the sum of the above:

$$KWUSE = (KWPUMP + KWREFR + KWLAS + KWIC + KWHVO + KWRCWO) * AVAIL + KWLIO ,$$

where AVAIL = the average plant availability.

The installed power requirement represents that which must be handled by the electrical distribution system and exceeds the average power usage. In this manner the system can handle those instances in which the instantaneous power use is above the average usage. In essence the installed power requirement must be sized to handle

everything running at once. A composite power factor of 95% and the availability is used to calculated the needed overdesign:

$$KWCAP = KWUSE/(0.95 * AVAIL) .$$

The turbines produce power which is assumed to be usable by the facility, hence the power which is purchased is the difference between the power use above and the turbine production. In many instances the facility will produce net power which can be sold to obtain a credit.

$$KWNET = KWUSE - (WTURB * 0.745) * 0.85 ,$$

where:

WTURB = the turbine work in horsepower,

0.745 converts hp to kW, and

0.85 is a turbine efficiency.

The power cost is calculated as follows:

$$POWERC = KWNET * 8760 * CPOWER ,$$

where CPOWER is the unit cost of electrical energy in $/kWh.

Steam costs: 600 psig steam is assumed to be available on-site at a cost of $2.90/1000 lb. The steam requirement SREQ in lb/yr is calculated in the energy management code.

$$CSTMME = (SREQ/1000) * 2.90 .$$

Plant makeup cooling water: Nearly all the electrical energy consumed in the plant, especially that from energy inefficient lasers, is eventually dissipated as heat which must be removed by a cooling water system. The makeup cooling water requirement scales with the plant power consumption.

$$CCW = (KWUSE/KWUSEB) * 847 .$$

Plant compressed air: Compressed air costs are assumed to scale with the plant throughput as follows:

$$CAIR = 25000 * (MOFLOW/MOFLWB) .$$

Other utilities: Other facility utility costs are assumed to scale with building area.

$$COTHL = 15000 * (ATOT/ATOTB) .$$

Total utility costs are calculated as the sum of the above.

$$CUTIL = POWERC + CSTMT + CCW + CAIR + COTHL .$$

4. Interest on working capital and inventories: The IOWC in this case consists of an interest charge of 10 percent of 2 months' worth of operating expense:

$$CIOWC = 0.1 * (2/12) * (CLABOR + CREPL + CMAINT + CUTIL) .$$

The syngas cleanup system has no significant holdup of feedstock materials, hence no in-process inventory investment. The total annual operating cost exclusive of amortization consists of the following sum:

$$CAN1 = CLABOR + CREPL + CMAINT + CUTIL + CIOWC .$$

Amortization. Capital recovery is assumed to take 25 years at an interest rate of 10 percent. The resultant capital recovery factor of 0.1102 per year has been used in the past for the evaluation of government financed energy projects. The annual amortization charge is calculated as:

$$CAMORT = 0.1102 * CTOT ,$$

where CTOT = the total capital cost.

Total annualized costs. The annual production cost is calculated from the two components above:

$$ANCOST = CAN1 + CAMORT .$$

Calculation of unit cost. The unit cost is obtained by the quotient of the above total annualized cost and the productivity. In this case we are interested in the cost per unit of methanol rather than the cost per unit of sulfur removed or the cost per unit of synthesis gas processed. Discussion of the figures of merit will be considered in a later subsection. One portion of the economic model has yet to be discussed, and this is the reliability-availability-maintainability (RAM) model.

RAM model. The overall onstream fraction or plant availability depends on the reliability of the components which comprise the plant operating system. Since this application consists of sequential steps, it is assumed that the reliability algorithms for series connected elements apply. The total plant availability can be calculated as the product of the following single element availabilities (Table I.6), most of which have constant values.

Table I.6

Component Availabilities

Component	FORTRAN Name	Availability
Compressor	AVCOMP	0.999
Turbine	AVTURB	0.995
Nozzle	AVNOZ	0.993
Utility and support	AVUTIL	0.999
Laser and optics	AVLAS	(variable)
Collector	AVCOLL	(variable)

Failure of the optical elements shuts down the laser system, thus the availability of the laser system depends on the lifetime, OPTLIF, and the mean time to restore, OPTREP, of the optical unit:

$$\text{AVLAS} = \frac{\text{OPTLIF}}{\text{OPTLIF} + \text{OPTREP}} .$$

The collector availability depends on a similar relationship:

$$\text{AVCOLL} = \frac{\text{COLLIF}}{\text{COLLIF} + \text{COLREP}} .$$

The lifetime for the optical unit depends on the laser fluence as follows:

$$\text{OPTLIF} = 25/\phi_{fo} ,$$

where ϕ_{fo} is the estimated laser fluence in joules/cm^2.

The relation is illustrative of the fact that RAM elements in a process can depend on basic process science attributes.

The overall availability is calculated as follows:

```
AVAIL = ABERNY * (AVCOMP ** 4) * (AVTURB ** 3) *
        AVNOZ * AVUTIL * AVLAS * AVCOLL .
```

The power terms reflect the fact that for the baseline there are three and four turbines and compressors in series, respectively. ABERNY is an operational availability of 0.987 inserted to account for facility outages due to non-equipment failures, i.e., labor problems, power failures, etc.

Calculation of the figure of merit. Since the photochemical sulfur removal process is part of an overall methanol production scheme, the most obvious figures of merit will be the incremental and total costs of

methanol produced by a plant with the above sulfur removal system installed instead of ZnO catalyst guard beds. The numerator term for the incremental unit cost of methanol has been calculated above as the annual operating cost. The desired denominator term is the amount of methanol produced or methanol productivity. This value is merely a function of the synthesis gas throughput.

$$TCH3OH = FRACTM * FEEDKG * AVAIL$$

where:

FRACTM = the fraction of syngas converted to methanol (= 1.0 for this type of recycle reactor),

FEEDKG = the design throughput or kilograms of syngas processed per year (a fixed input, 6.038×10^8 kg/yr in baseline), and

AVAIL = plant onstream fraction or availability.

For the baseline plant the methanol output is 76 tons/hr or 6.66×10^5 tons/yr.

It should be noted that the design syngas throughput and the sulfur decontamination factor (50) are kept constant for all cases modeled. The equipment and utility requirements, hence operating costs, needed to meet these goals vary widely, depending on other input parameters to the process model. The actual productivity or denominator term of the unit cost (tons of methanol per year) varies only slightly, i.e., due only to availability or methanol conversion changes. The design productivity is assumed constant.

For most cases involving off-baseline operation, degraded performance does not show up in the productivity term, rather it emerges as

significantly increased operating cost due to the additional equipment, energy, personnel, and materials. This conforms to the DTFR modeling format discussed in Chapter V. The incremental unit cost is calculated as

$$\text{CUNIT} = \text{ANCOST/TCH3OH} .$$

Calculation of the total methanol unit cost requires knowledge of the annual synthesis gas feedstock cost and the annual cost of operating the conventional methanol synthesis plant. The latter cost should not include a ZnO or photolytic sulfur removal system. The acid gas removal (Rectisol or Benfield plant) and the bulk sulfur recovery operation (Claus plant) should be included, however. Fortunately, the EPRI study[121] cited previously contained most of this methanol plant cost information. The synthesis gas feedstock cost is a function of its heating value. The 2-to-1 ratio (H_2 to CO) syngas is considered to be a "medium BTU" gas (300 BTU/standard cubic foot) available at $7.20 per million BTUs. This translates to a cost of $145 per ton or $0.16 per kg of syngas (or methanol), assuming the conversion for $2H_2 + CO \rightarrow CH_3OH$ is unity.

The total annualized cost, which includes capital recovery, for the methanol plant is assumed constant at $14.25 million. This cost does not include ZnO desulfurization units or the Claus plant for reclaiming sulfur from the primary (Rectisol or Benfield) sulfur removal units. The unit cost of methanol assignable to the synthesis plant is $23.44 per ton or $0.026 per kg methanol.

The operating costs for a Claus plant are estimated to constitute 5%

of the methanol plant above, thus adding another $7.27 per ton or $0.008 per kg methanol.

To the total of the syngas feed, methanol synthesis gas, and Claus plant unit costs can be added the incremental unit cost of the photolytic desulfurization facility. The resulting total unit cost of methanol is the figure of merit of predominant interest. Other figures of merit useful to the evaluator are the following:

1. Percentage change in unit cost of methanol from that of a plant with conventional ZnO sulfur removal.
2. Unit cost of gas handling (compression, nozzle, turbines, etc.).
3. Unit cost of photon energy (lasers and optics).
4. Unit cost per kg of sulfur removed.
5. Unit cost of synthesis gas processed.

Values for these will be presented in the baseline data in the next subsection.

Process baseline summary tables. The following tables (Tables I.7, I.8 and I.9 and Figure I.15) present the baseline design conditions for the photolytic syngas cleanup system. Such data give the reader a better sense of the physical size and other attributes of the system. These single values comprising the baseline are divided into several categories.

Following these is a set of tables (Tables I.10 through I.14) describing the economics of the baseline, i.e., the capital, operating, and unit costs and the baseline performance.

Table I.7

Photolysis Zone Baseline Conditions

Laser Beam Data	
*Beam height (HIZ)	1.0 cm
Beam width (WIZ)	2.0 cm
Irradiation zone length (L)	788.2 cm
Irradiation zone cross-sectional area	2.0 cm^2
Irradiation zone volume	1576 cm^3
Syngas Conditions in Irradiation Zone	
*Total pressure (TORR)	760 torr
*Temperature (TEMP)	273 K
Gas velocity	54706 cm/sec
*Mach number (FRMACH)	1.0
H_2 to CO mole ratio	2
Average molecular weight	10.76 g/g-mole
Flow rate	1.43×10^9 lb/yr
	6.47×10^8 kg/yr
	4.8×10^{10} scf/yr
	9.14×10^4 scfm
Molecular density	2.69×10^{19} molecules/cm^3
Heat capacity ratio (γ)	1.406
Pre-Photolysis H_2S Conditions in Irradiation Zone	
H_2S concentration	5 ppm
H_2S molecular density	1.344×10^{14} molecules/cm^3
Molecules H_2S/sec	5.794×10^{21}/sec
H_2S partial pressure	3.8×10^{-3} torr
S molar flow rate	3.034×10^5 g mole S/yr
*Photon absorption cross section (SIGMA)	1×10^{-17} cm^2
Photolysis Zone Laser Light Characteristics	
UV Wavelength (λ)	210 nanometers
Photon flux (ϕ_o)	5.2×10^{17} photons/cm^2
Fluence (ϕ_{fo})	0.495 joules/cm^2
PRF	2.74×10^4 Hz
Pulse duration	10^{-7} sec
Beam Intensity	9.9×10^6 watts/cm^2
Average output power required for photolysis	2.71×10^4 watts
Energy per laser beam pulse	0.991 joules
Photon rate	1.5×10^6 Einsteins/yr

*Designates uncertain X_i input variable to be used in MVSS

Table I.7 (Continued)

Photolysis Reaction Performance	
Limiting yield, θ_{lim}	0.9947
Yield at L = 788 cm, θ_L	0.9848
Average yield, θ_{ave}	0.99056
Photon utilization	20%
Post-Photolysis Conditions and Performance	
*Total pressure (PCOLLF)	760 torr
*HS-HS recombination rate constant, k (RECRAT)	3×10^{-11} cm^3/ molecule-sec
HS-HS reaction half-life ($t_{1/2}$)	2.5×10^{-4} sec
Post-photolysis collection yiel(θ_{pp})	0.99
Fraction recombined	0.01
HS fragment transit time	5×10^{-6} sec
HS-HS collisional cross section (σ_{HS})	3.5×10^{-8} cm^2
HS-HS mean free path	1.38 cm
Time between HS-HS collisions (t_{coll})	3.3×10^{-5} sec
Collector pore diameter (d_{tube})	0.211 cm
Total Stage Performance	
Total H_2S decomposition yield including post-photolysis effects (θ_{tot})	0.9806
Decontamination factor	51.9

*Designates uncertain X_i input variable to be used in MVSS

Table I.8

Equipment Specifications for Baseline Case

Laser System	
PRF per single laser head	1.25 kHz
Maximum power per laser head	7.5 kW
Number of timed laser sets	22
Heads per laser set	1
Actual laser head power	1.238 kW
*Overall laser efficiency (EFF)	0.01
Wall plug power (total laser system)	2.71 MW
Nozzle System	
Plenum pressure	1441 torr
Plenum temperature	328.4 K
Throat area	788.2 cm^2
*Throat height (HIZ)	1 cm
Nozzle length	788.2 cm
Critical pressure ratio	0.527
Maximum possible Mach number	2.22
*Operating Mach number (FRMACH)	1.0
Turbine System	
Inlet pressure (first turbine)	31.6 atm
Outlet pressure (third turbine)	1.9 atm or 1441 torr
Turbine inlet temperature	580 R
Turbine outlet temperature	442 R
Reheat requirement per turbine	1.44×10^7 Btu/hr or 1.26×10^{11} Btu/yr
Total turbine work (3 turbines)	16970 hp
Electric power production (3 turbines)	10746 kW
Heat exchanger tube area (per turbine)	128 ft^2
Compressors	
Number required	4
Inlet pressure (first compressor)	1 atm
Outlet pressure (fourth compressor)	76 atm
Total energy requirement, electrical equivalent	37936 hp 24023 kW
Heat production (total)	8.51×10^{11} Btu/yr
Portion of heat production used to reheat syngas	2.19×10^{11} Btu/yr
Heat exchanger (intercooler) load (total)	6.32×10^{11} Btu/yr
Heat exchanger tube area required	2966 ft^2
600 psig, 1000F steam requirement to drive compressors	2.16×10^9 lb/yr

(See Table I.2 for individual compressor requirements)

Table I.8 (Continued)

Other Energy Management	
600 psig, 1000F steam required to reheat syngas before methanol synthesis	1.26×10^{11} lb/yr
Heat exchanger load for reheat	1.56×10^{7} Btu/hr
Total centrifugal pump capacity	4.71×10^{3} gpm
Electric power required for pumping	46.6 kW
Refrigeration requirement for compressor coolant	3089 hp or 2423 kW
Plant Electric Power	
Lasers	2710 kW
Centrifugal coolant pumps	47 kW
Refrigeration	2423 kW
Instrumentation and controls	100 kW
Lighting	29 kW
Heating and ventilation	139 kW
Recirculating water system	783 kW
Total operating power consumed	6231 kW
Electricity produced from turbines	10746 kW
Net power production	4515 kW
Total installed capacity (power consuming hardware only)	6852 kW
Facility Layout	
Plenum, irradiation zone, collector	1543 ft^2
Expansion turbines, reheaters, and generator	3800 ft^2
Compressors, coolers, and motors	4200 ft^2
Laser system including power conditioning	880 ft^2
Beam handling equipment	440 ft^2
Collector refurbishment	2500 ft^2
Syngas storage tanks	1200 ft^2
Process support	1250 ft^2
Total add-on building area	15813 ft^2

*Designates uncertain X_i input variable

Table I.9

Cost and Reliability Inputs for the Baseline Case

Laser System	
*Capital cost per watt (CCPWAT)	$500/output watt
*Operating costs per watt (OCPWAT)	$100/output watt
Sulfur Collector	
*Collector lifetime (COLLIF)	12 hr
*Optical unit cost (COUNIT)	$800/unit

*Designates uncertain X_i input variable to be used in MVSS

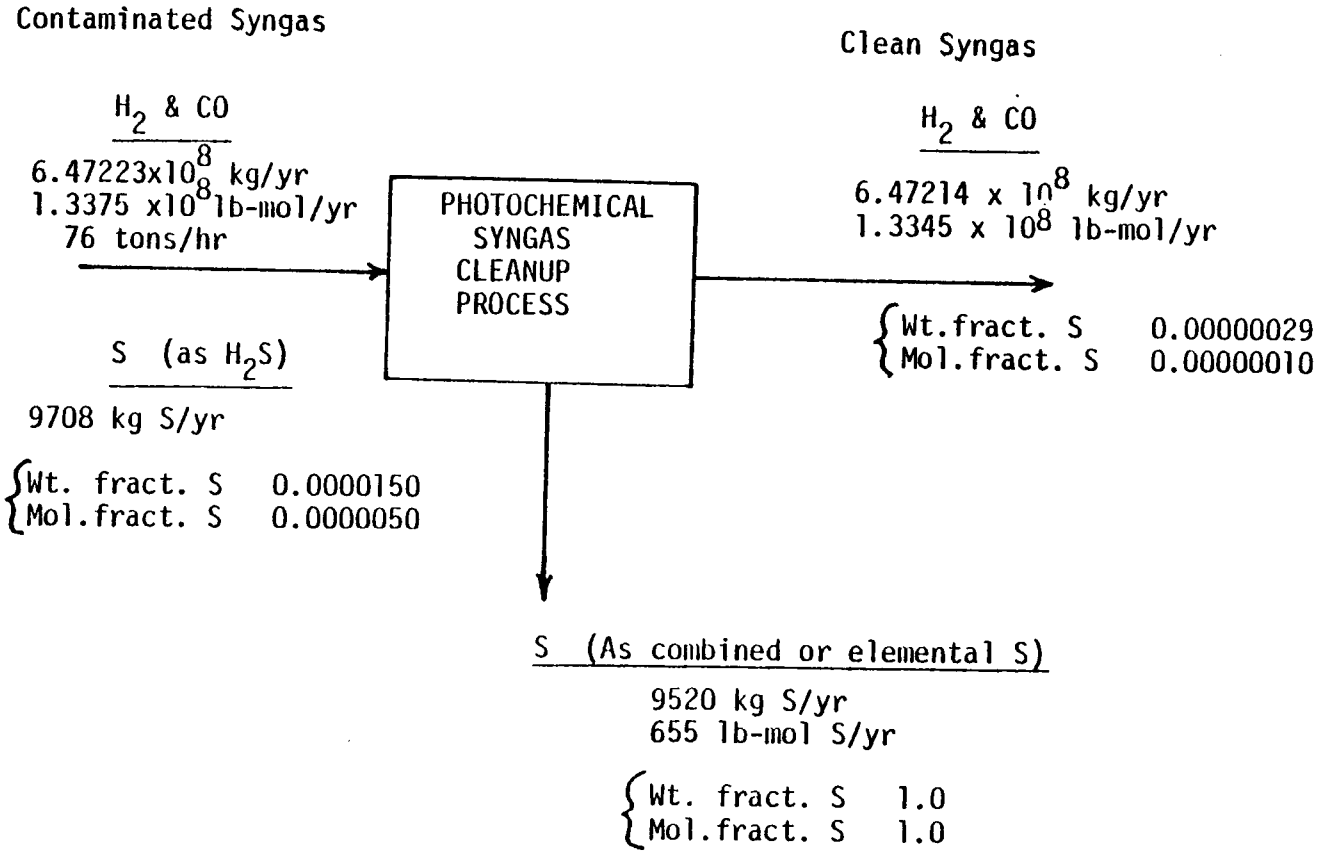


Figure I.15

Baseline Material Balance

Table I.10

Total Capital Cost of Baseline Photolytic Sulfur Removal Facility
(Thousands of Dollars)

Nozzle, plenum, discharge section, and initial collector	157.6
Spare collector units	8.0
Laser system	13,550.1
Beam transport system	2,710.0
Optical multiplexer	100.0
Spare optical units	4.0
Expansion turbines	649.5
Turbine reheaters	70.0
Turbine generators	405.9
Compressors	4,707.3
Compressor steam turbines	1,400.4
Compressor coolers	94.9
Refrigeration for compressor coolant	552.6
Heat exchanger for post compression reheat	5.8
Storage tank for plenum syngas	233.7
Heat exchanger coolant pumps	87.9
Cooling water system for lasers	162.7
Instrumentation and control	100.0
Pre-operational checkout	115.4
Outside utilities (including switchgear)	2,289.3
Special shops (including collector refabrication)	50.0
Electrical distribution system	40.0
System piping	17.3
Building	1,897.6
Subtotal	29,410.0
Engineering at 25% of direct costs	7,352.6
Subtotal	36,762.6
Contingency at 41.3% of above	15,185.6
Subtotal	51,948.2
Interest during construction at 10%	5,194.8
Total capital cost	57,143.0

Table I.11

Operating Costs: Labor and Steam

Category	No. of Employees* M	WT	WC	H	Labor Cost ($ Thousands)
Staffing Table and Costs for Five-Shift Operation					
Supervisory	5				170.000
E-O System repair and collector refurbishment				15	300.000
Technical support		1			22.000
Clerical support			1		14.000
Total cost for a staff of 22					492.000
Steam Requirements					
Steam requirements and annual costs at 2.90 per thousand lb:					
Steam turbine driven compressors	0.216×10^{10}				6,274
Reheat of syngas prior to MEOH reactor	0.126×10^{9}				365
Total steam cost					6,639

*M: monthly
WT: weekly technical
WC: weekly clerical
H: hourly

Table I.12

Total Annual Operating Costs
(In Thousands of Dollars)

Labor Costs:		
Total direct labor costs for a staff of 22	492.0	
Fringe benefits at 25%	123.0	
Subtotal	615.0	
Contingency at 20%	123.0	
Total Labor Costs		738.0
Replacement and Material Costs:		
142 optical units @ $800 each (incl. 50% cont.)	170.9	
681 collector units @ $801 each (incl. 30% cont.)	709.2	
Additional work materials (incl. 20% cont.)	51.6	
Total Replacement and Material Costs		931.7
Maintenance Costs:		
Lasers (@ $100 per watt-yr)	2710.0	
Other plant maintenance	100.0	
Total Maintenance Costs		2810.0
Utility Costs:		
Electric power @ 0.03 per kWhr	-1186.6	
Steam	6638.9	
Cooling water	0.8	
Plant air	25.0	
Other utilities	14.4	
Total Utility Costs		5492.5
Interest on Working Capital		166.2
Subtotal Annual Costs		10138.4
Amortization of Capital ($57,143,278 at capital recovery of 0.1102)		6297.2
Total Annual Costs		16435.6

Table I.13

Annual Baseline Production

Kilograms of syngas feed processed or methanol synthesized	603.8 million kg/yr
Tons of syngas processed or methanol synthesized	76 tons/hr 1823.8 tons/day 6.65×10^5 tons/yr
Plant availability or on-stream fraction	0.9329
Design plant capacity	81.46 tons/hr

Table I.14

Calculation of Baseline Methanol Cost

	Methanol	
	$/ton	$/kg
2:1 syngas (300 Btu/scf @ $7.20 per MM Btu)	145.38	0.160
Methanol plant (excluding Claus plant and ZnO S removal @ annual cost $0.14E + 08/yr)	23.44	0.026
Claus sulfur recovery plant (5% of syngas cost)	7.27	0.008
Laser H_2S removal (baseline)	24.69	0.027
Total Costs	200.78	0.221

Other Baseline Figures of Merit

Unit Costs:	
$/mole of photons	4.42
$/EV-mole of photons	0.75
Photon cost per mole of S removed	22.3
$/mole H_2S in feed (gas handling)	24.2
Additional $/kg methanol produced	0.027
Percent additional cost	14.02
$/kg of S removed	1726.
At a stage cut of	0.981
$/thousand scf of syngas irradiated	0.342

Correction Factors to Adjust Figures of Merit

The model described is considered sufficiently detailed that there was no need to include adjustment factors on the figures of merit in the baseline case. In order to illustrate the use and effects of these factors in uncertainty analysis, an example MVSS will be shown which includes the following ranges on the performance discount factor, F_{PD}, and the capital cost growth factor, F_{CCG}:

F_{PD}	0.6 - 1.0
F_{CCG}	1.0 - 1.8

Evaluation of Uncertainty

Selection of Assessment Model Inputs and Their Distributions for Uncertainty Analysis

The selection of variables to be treated as uncertain inputs should be made on the basis of which variables have the highest leverage on the figure of merit and also have significant uncertainty in their values. Familiarity with the details of the assessment model is necessary in order to choose which quantities constitute input variables. The determination of the subset of high leverage variables, which also have significant enough uncertainty to cause material uncertainty in the figure of merit, requires detailed knowledge of the process and its supporting data base. Fifteen user-determined variables were identified for which values were needed in order to complete a design and rough cost estimate for the process baseline. Table I.15 lists these variables, their FORTRAN names, descriptions, units, and baseline

Table I.15

Input Variables for Photolytic Syngas Cleanup Model

Description	FORTRAN Name	Units	Class/Subclass	Baseline Value	% Change in Sensitivity Incremental Methanol Cost / % Change in Variable (at baseline)
Performance Drivers:					
Irradiation zone total pressure	TORR	torr	Process Science & Chemistry/Scaling	760	-0.15
Irradiation zone gas temperature	TEMP	K	Process Science & Chemistry/Scaling	273	0.14
Collection zone pressure as fraction of irradiation zone total pressure	PCOLLF	dimensionless	Process Science & Chemistry/Scaling	1.0	-0.25
H_2S absorption cross section for 193 nm UV laser radiation	SIGMA	cm^2	Process Science & Chemistry/Natural	1×10^{-17}	-0.70
HS-HS recombination reaction rate constant	RECRAT	cm^3/molecule-sec	Process Science & Chemistry/Natural	3×10^{-11}	0.0
Velocity of syngas expressed as the Mach number	FRMACH	dimensionless	Process Science & Chemistry/Scaling	1.0 (Mach 1 = 54700 cm/sec)	0.45
Irradiation zone height	HIZ	cm	Process Science & Chemistry/Scaling	1.0	0.39
Irradiation zone width	WIZ	cm	Process Science & Chemistry/Scaling	2.0	-0.013
H_2S concentration in syngas	PPM	parts per million by volume	Process Science & Chemistry/Scaling	5.0	0.3
Synthesis gas feed rate	FDRQKG	kg/yr	Process Science & Chemistry/Scaling	6.038×10^8	0.6

Table I.15 (Continued)

Descr.	FORT. Name	Units	Class/Subclass	BL Value	BL Slope
Cost Drivers:					
Laser system efficiency	EFF	dimensionless	Hardware Performance	0.01	-0.05
Collector lifetime	COLLIF	hrs	R.A.M.	12	-0.065
Laser cost per watt of output	CCPWAT	$/watt	Equipment Cost	500	0.23
Cost per optical unit (capital and replacements)	COUNIT	$/unit	Equipment Cost or Operating Cost	800	0.01
Laser operating costs per output watt exclusive of power (parts, maintenance labor)	OCPWAT	$/watt-yr	Operating Cost	100	0.165

values. The variable classification as described in Chapter XIII is also given. It is from this list that the array, X_i, of uncertainty variables are chosen.

Selection of which variables are to constitute uncertainty inputs. The decision as to which of these variables become inputs to the uncertainty analysis depends on whether each has enough performance or economic leverage to significantly affect the figure of merit (in this case the incremental cost associated with the unit cost of methanol incurred by deploying the photolysis system). In order to make this determination, single value sensitivity studies (SVSS) must be made on each input variable and the ratio (% change in figure of merit/% change in input) examined in the range of interest. By expressing the above in terms of percentage changes from baseline and plotting on common axes, as in Figures I.16 and I.17, the important process drivers become apparent. Figure I.16 shows the sensitivities for the performance-related variables, and Figure I.17 shows the sensitivities for the economic-related variables. Table I.15 lists the nominal values of the slopes or derivatives of these curves at the baseline. The higher the absolute value of a particular slope, the more the variable drives the unit costs. It can be seen that the H_2S absorption cross section (SIGMA), the irradiation zone and collector pressures (TORR and PCOLL), and the nozzle-related parameters (HIZ and FRMACH) are the dominant performance drivers. The plant syngas feedrate (FDRQKG) and input H_2S concentration (PPM) are important drivers; however, since the photolysis step is part of a total methanol production system, these variables have values fixed by the rest of the production system. As expected, unit

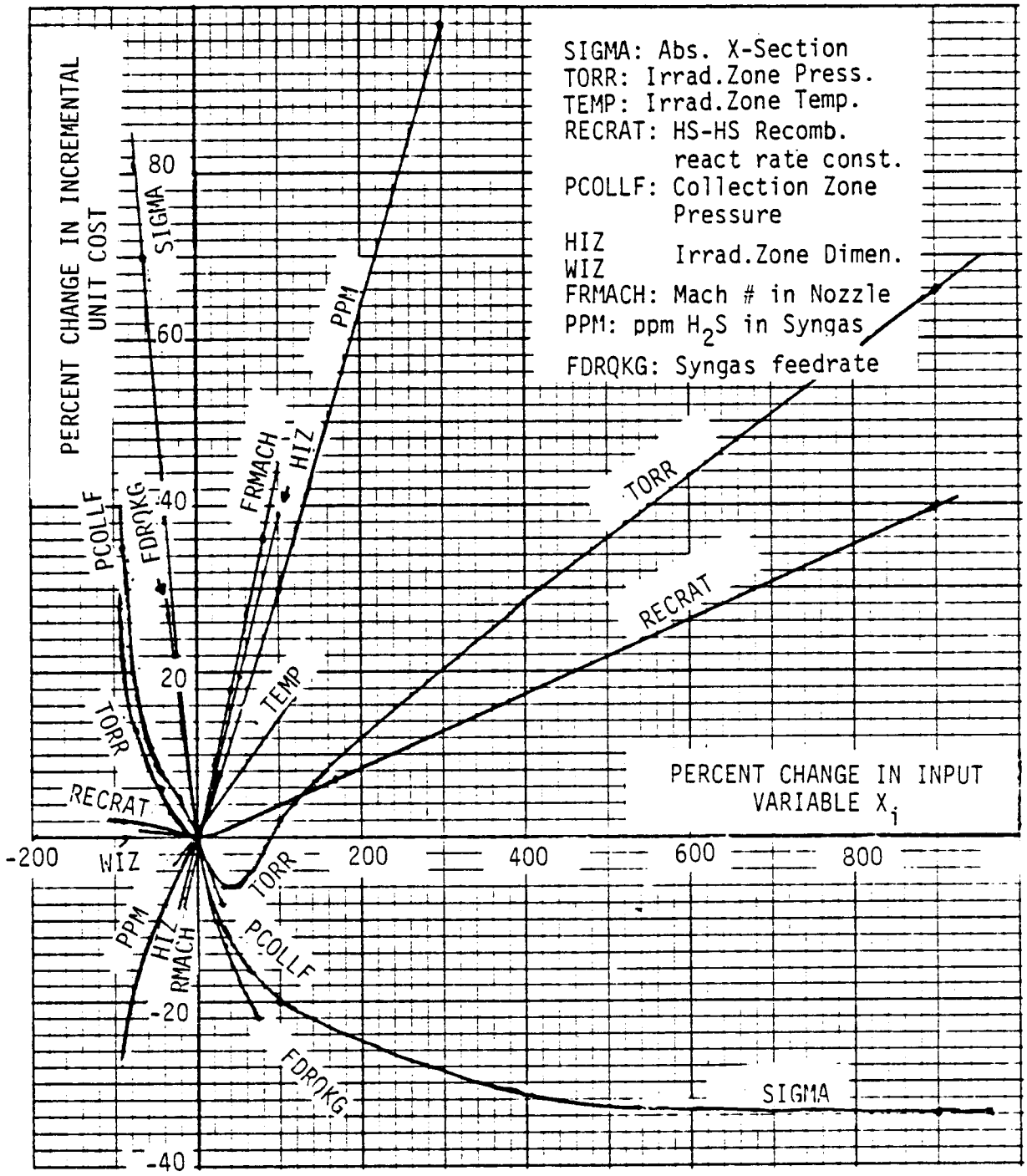


Figure I.16

Sensitivity of Incremental Methanol Desulfurization Unit Cost to Performance and Design Variables

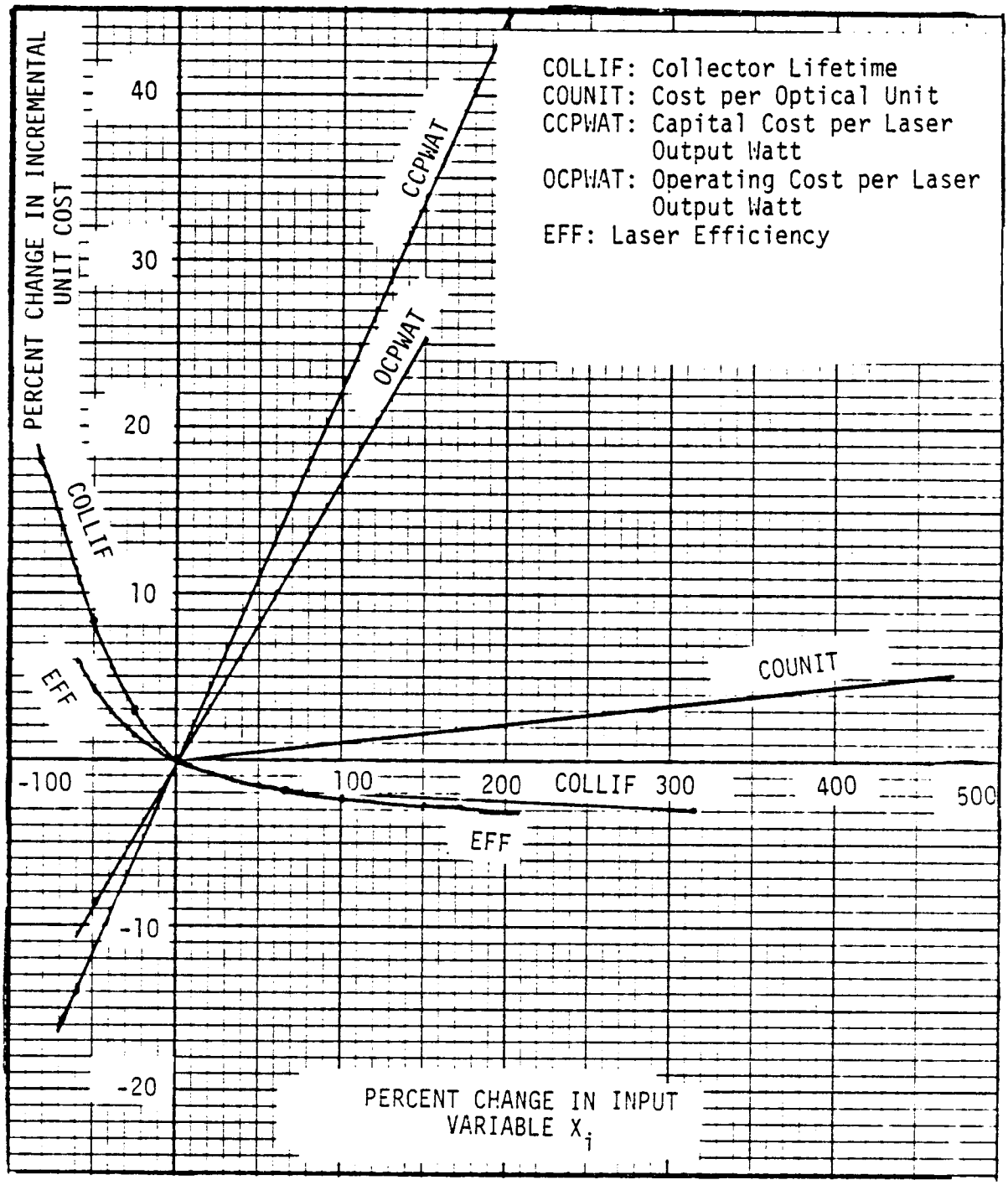


Figure I.17

Sensitivity of Incremental Methanol Desulfurization Unit Cost to Cost Variables

costs decrease with a larger plant and lower decontamination requirements. For uncertainty analysis, however, one is concerned with the risk in attaining a given fixed decontamination requirement at a fixed plant size, i.e., maintaining constant performance.

Figure I.17 shows that the laser related capital and operating costs constitute the major cost drivers. The next step is to select the input variables for uncertainty analysis from the fifteen considered in SVSS. From the previous Figure I.16 one can see that the variable WIZ (irradiation zone width) has a small slope, hence will not be a cost driver. Since the required decontamination and feedrate are to be held constant, they can also be eliminated as uncertainty variables. The rationale for the selection of ranges and input probability distributions for the remaining twelve uncertainty input variables will now be considered.

Selection of uncertainty input ranges and probability distributions. For projects under serious consideration by a corporate or private organization, this step is often the most difficult and subjective part of the entire evaluation. It usually requires assembling a group of experts for a peer review process or some more formalized method of technology assessment. The example process, photolytic syngas cleanup, has not been subjected to extensive economic analysis or peer review within any organization. The calculation made by Chen and Borzileri[122] at Livermore was of the "back-of-the-envelope" type and did not consider uncertainties or integration of the process into a methanol production plant. For these reasons the input ranges and distributions to be discussed are

not the result of a group's combined opinion but are the result of the authors' educated but still subjective opinion. This is not regarded as a serious shortcoming in this case, since the purpose of this section is to illustrate application of the overall methodology rather than make an extremely rigorous evaluation of photolytic synthesis gas cleanup. The approach used here will be to discuss each of the twelve uncertainty analysis input variables separately and discuss the modes of thought used in assigning ranges and distributions to each. Table I.16 gives a summary of the ranges and distributions for each. Before considering each variable, a few general observations will be made.

For many variables, the endpoint values for the distribution range represent optimistic and pessimistic values. All of the distributions considered here have one of their defining points as the mode or most likely value in the distribution. This mode value need not correspond to the baseline value for the variable in question; however, for ten of the twelve variables here considered, the two are identical. This situation often arises since MVSS input parameter distributions are usually determined by a group different from the proponent organization which defines the baseline. In some cases the baseline value may even lie outside the range of an input distribution for a given variable. In the following discussion, performance-related variables will be considered first.

1. Absorption cross section (SIGMA). The cross section for the absorption of UV is a measured variable which for a single set of process conditions can be determined with the precision of a few percent. (Since photolysis conditions are known to affect the value of σ_{H_2S}, but the

Table I.16

Ranges and Distributions for Uncertainty Analysis Inputs

No.	Description	FORTRAN Name	Baseline Value	Type of Distribution	Minimum	Mode	Maximum
	Variables in Model (MVSS #1 & #2)						
1	Absorption Cross Section, σH_2S	SIGMA	1×10^{-17} cm^2	Log-Triangle	0.1×10^{-17} (P)†	0.75×10^{-17}	5×10^{-17} (O)
2	Irradiation Zone Temperature	TEMP	273 K	Triangular	250 (O)	273	400 (P)
3	Irradiation Zone Pressure	TORR	760 torr	Triangular	100	760	1520
4	Mach Number	FRMACH	1.0	Triangular	0.9 (O)	1.0	1.8 (P)
5	Irradiation Zone Height	HIZ	1.0 cm	Triangular	0.5 (O)	1.0	2.0 (P)
6	Collector Pressure Multiplier	PCOLLF	1.0	Triangular	0.2 (P)	1.0	1.2 (O)
7	Recombination Reaction Rate	RECRAT	3×10^{-11}	Triangular	1×10^{-11} (O)	3×10^{-11}	5×10^{-11} (P)
8	Collector Lifetime	COLLIF	12 hr	Triangular	8 (P)	12	20 (O)
9	Optical Unit Cost	COUNIT	$800	Triangular	1000 (O)	2000	3000 (P)
10	Laser Capital Cost per Watt	CCPWAT	$500/watt	Triangular	300 (O)	500	800 (P)
11	Laser Operating Cost per Watt-Year	OCPWAT	$100/watt-yr	Triangular	50 (O)	100	200 (P)
12	Laser Efficiency	EFF	0.01	Triangular	0.005 (P)	0.01	0.025 (O)
	Figure-of-Merit Adjustment Factors (MVSS #2 Only)						
1	Performance Discount Factor	F_{PD}	1.0	Triangular	0.6 (P)	1.0	1.0 (O)
2	Capital Cost Growth Factor	F_{CCG}	1.0	Triangular	1.0	1.0	1.8 (P)

†SVSS Results: (O) = Optimistic (lower unit cost)
(P) = Pessimistic (higher unit cost)

functional form of the relationship is unknown, the range on σ_{H_2S} has been made significantly larger than the measurement error bars.) A range which spans nearly one order of magnitude has been chosen since it is likely that the value of σ_{H_2S} under any process conditions handled by the model will fall in this range. A log-triangle distribution was chosen to handle this order of magnitude range and force the mode to more nearly approximate the median. Note that the mode value used is conservative, i.e., pessimistic, relative to the single point value utilized for the baseline case.

2. Irradiation zone temperature (TEMP). It is proposed that the gas can be easily handled in the range of 250 to 400 K without the addition of new process support equipment. Since this selection of possible operating temperatures is subjective, the triangular distribution and its simple formulation is sufficient for use here.

3. Irradiation zone pressure (TORR). This variable is important in that it fixes the molecular density of the H_2S irradiated, hence also the area of nozzle throat required. The low value of 100 torr is in the range of actual experimentation; the high range is limited by the fact that recombination effects will begin to dominate. The mode value of 760 torr is close to the optimum pressure determined by SVSS studies. A triangular distribution was deemed a suitable representation for these data.

4. Mach number (FRMACH). The gas velocity affects the laser repetition rate and the nozzle sizing. The lower value of 0.9 was chosen since it would be difficult to operate such a nozzle at a velocity much below Mach 1. The upper limit of 1.8 falls just below the maximum

possible Mach number which itself is a function of gas properties and shock wave phenomena. The triangular distribution with a mode equivalent to the base case Mach number of 1.0 has been chosen.

5. Irradiation zone height (HIZ). This variable is an important determinant of laser beam and nozzle size. The lower limit of 0.5 is limited by beam propagation considerations and the upper limit by laser optics constraints. The triangular distribution is again considered appropriate.

6. Collector pressure (PCOLLF). This multiplier relates the collector pressure to the irradiation zone pressure. Both the upper and lower limits are imposed by aerodynamic considerations for flow downstream of the nozzle throat. Since it is most likely that the collection zone and irradiation zone pressures will be equal, a triangular distribution with a mode of 1.0 is chosen.

7. Recombination reaction rate constant (RECRAT). This measured quantity depends on process conditions to an unknown degree, hence a range was chosen to include a wide range of possible operating conditions. A triangular distribution centered about the baseline value of 3×10^{-11} was chosen.

8. Sulfur collector lifetime (COLLIF). The collector lifetime will depend on such unknowns as the sulfur particle size, degree of abrasion, degree of chemical attack, and the materials of construction. In any case, changeout will be required in a matter of a few hours of process operation. A range of 8 to 20 hours encompassed by a triangular distribution with a mode of 12 hours is felt sufficient.

9. Optical unit cost (COUNIT). Since the design of the optics is in the conceptual stage at best, a wide range was chosen. In this case the baseline cost of $800 was felt so optimistic that it fell outside the MVSS range of $1000 to $3000 per unit. A mode cost of $2000 for a triangular distribution was felt reasonable.

10. Laser capital cost per watt (CCPWAT). Projections made for RGH lasers operating in the UV indicate that $500 per output watt is a reasonable development goal. Better than expected economies of scale could lower this unit cost and development difficulties could increase this unit cost markedly. A range of $300 to $800 per watt is felt to be realistic. A triangular distribution with a mode of $500 per watt is used.

11. Laser operating costs per watt (OCPWAT). The same general comments as 10, above, apply with the exception of the ranges; $50 to $200 per output watt year is considered reasonable. A triangular distribution with a mode of $100 per watt year is considered reasonable.

12. Laser efficiency (EFF). Values for this parameter are based on both laboratory results and development projections based on theoretical calculations. The mode (and baseline) value of 0.01 represents the likely efficiency to be achieved in a future laser system. The lower limit is closer to actual results to date. The upper limit is imposed by scale-up and theoretical limitations. A triangular distribution is again considered appropriate.

Distribution for figure-of-merit adjustment factors. After the above case, which consists of twelve input variables, was set up and run with the similator, an additional case (MVSS #2 in Table I.16) was run

which included two figure of merit adjustment factors. This case was run for the purpose of illustrating the effect of these factors on process unit cost uncertainty. For MVSS Case #2 triangular distributions were used for the probability distributions for the two figure-of-merit adjustment factors. For F_{PD} and F_{CCG} the mode of the distribution also represents baseline, which means that the author believes that the baseline design ($F_{PD} = 1$, $F_{CCG} = 1$) is more likely to be attained than not; however, the risk associated with not meeting the baseline will be increased over that predicted by the model alone. For the performance discount factor the minimum of 0.6 represents the lower limit F_{PD} determined earlier. No maximum value of F_{PD} above 1.0 was calculated since no existing backups to the basic photolysis process were identified. The capital cost-growth factor, F_{CCG}, has its maximum set at 1.8 for illustrative purposes. No F_{CCG} value less than 1.0 was utilized since the author again visualizes no alternative backup process with which lower costs can be attained. The input statistics associated with each distribution appear in Table I.16.

The next section discusses interpretation of the results obtained by submitting the above uncertainty input data (with and without figure-of-merit adjustment factors) to the Monte Carlo code. The actual computer input data set for this photochemical example is shown in Appendix K.

Estimation of Economic and Technological Uncertainties Via Monte Carlo Simulation.

This step is not process specific and its associated methodology was described in Chapter XIII. The FORTRAN listing for the actual Monte

Carlo driver code used in simulation is included in Appendix M. The instructions for its use appear in Appendix L.

Interpretation of Analysis Results

Interpretation of Simulation Histograms and Statistics

Figure 9.9 shows a histogram representing a probability density function for an output figure of merit, in this case the unit production cost ($/ton) of methanol with a photolytic sulfur removal system. All twelve uncertain inputs are factored into this MVSS. The effects of figure-of-merit adjustment factors are not included. As expected a positively skewed bell-shaped histogram appears. The values of the pdf and cdf are tabulated along with the number of cases appearing in each bin. A total of 500 cases or iterations was generated to produce the histogram. As would be expected in a new process of this sort, the output histogram is skewed toward higher unit costs. The values lying between the 5 percentile and 95 percentile range from $196 to $306 per ton. The most probable or mode value can only be represented with the accuracy of the width of a bin, i.e., one can say that the methanol cost will most likely be between $195 to $200 per ton. The mean or expected value is calculated as $227 per ton. The standard deviation is useful for indicating the extent to which the results are dispersed about the mean and has a value of ~$40/ton.

Many cost items, such as compressors or laser heads, must be counted as discrete items, hence, the resulting capital cost function has a step-like appearance. By including such intermediate variables as capital cost subtotals in the simulator output list, actual plots for

such variables can be studied and the waviness of the total figure of merit plots explained. Figure I.18 shows output plots for other pertinent variables and figures of merit corresponding to the above MVSS.

For the remainder of this section, i.e., other MVSS, most of the uncertainty results will be given in tabular form; i.e., the 5 percentile, median (50 percentile), 95 percentile, mode, mean (μ), and standard deviation (σ) will be listed. The analysis above is depicted as MVSS No. 1 on Table I.17.

Relationship of Uncertainty Results to the Base Case

A single point methanol cost of $201 per ton was estimated for the baseline photolytic syngas cleanup process. The uncertainty analysis used somewhat more pessimistic values than baseline for two of the important input variables, SIGMA and COUNIT, and did not include figure-of-merit adjustment factors. The mean or expected value for the methanol cost from the histogram is $227 per ton. The baseline cost falls in approximately the 20 percentile of the uncertainty histogram. In essence this result implies that there is less than a 20% chance that achievement of the baseline cost will occur and that the risk of not achieving baseline is 80%. If two figure-of-merit adjustment factors (F_{PD} and F_{CCG}) are used in the uncertainty analysis a higher mean cost of $244 per ton is obtained from the resulting MVSS histogram (now based on 14 uncertain variables). In this case the chance of obtaining baseline ($201 per ton) is even smaller, i.e., less than 5%. The effects of simultaneously applying these two figure-of-merit adjustment factors is summarized in Table I.17 as MVSS No. 2 and the actual histogram is shown in Fig. 9.1. The upward trend of both the expected value (mean) and

STATISTICS FOR OUTPUT VARIABLE PHIOV (Output Laser Energy Fluence, ϕ_o)

MINIMUM 0.13729 MAXIMUM 4.2423

MEAN 0.92586 VARIANCE 0.58056 STD.DEVIATION 0.76195

PERCENTILES: 2.5% .155 5.0% .206 50.0% .678 95.0% 2.60 97.5% 3.15

500 POINT HISTOGRAM * = 1 POINTS

PROB	CUME	VALUE		
0.0440	0.0000	0.1000	22	**********
0.1080	0.0440	0.2000	54	**********
0.1180	0.1520	0.3000	59	**********
0.0860	0.2700	0.4000	43	**********
0.0880	0.3560	0.5000	44	**********
0.0720	0.4440	0.6000	36	**********
0.0720	0.5160	0.7000	36	**********
0.0580	0.5880	0.8000	29	**********
0.0340	0.6460	0.9000	17	**********
0.0400	0.6800	1.000	20	**********
0.0200	0.7200	1.100	10	**********
0.0200	0.7400	1.200	10	**********
0.0260	0.7600	1.300	13	**********
0.0300	0.7860	1.400	15	**********
0.0340	0.8160	1.500	17	**********
0.0220	0.8500	1.600	11	**********
0.0180	0.8720	1.700	9	**********
0.0100	0.8900	1.800	5	**********
0.0080	0.9000	1.900	4	**********
0.0040	0.9080	2.000	2	**********
0.0080	0.9120	2.100	4	**********
0.0060	0.9200	2.200	3	**********
0.0120	0.9260	2.300	6	**********
0.0100	0.9380	2.400	5	**********
0.0020	0.9480	2.500	1	**********
0.0020	0.9500	2.600	1	**********
0.0020	0.9520	2.700	1	**********
0.0080	0.9540	2.800	4	**********
0.0060	0.9620	2.900	3	**********
0.0040	0.9680	3.000	2	**********
0.0040	0.9720	3.100	2	**********
0.0060	0.9760	3.200	3	**********
0.0020	0.9820	3.300	1	**********
0.0020	0.9840	3.400	1	**********
0.0040	0.9860	3.500	2	**********
0.0040	0.9900	3.600	2	**********
0.0040	0.9940	3.700	2	**********
	0.9980	3.800		

(BL)

joules/cm^2

Baseline Value (BL)
0.5 j/cm^2

Figure I.18

Output Histograms for Other Figures-of-Merit

STATISTICS FOR OUTPUT VARIABLE PUTIL (Photon Utilization, fract. of photons abs.)

MINIMUM 8.73966E-03 MAXIMUM 0.61211

MEAN 0.13595 VARIANCE 1.15701E-02 STD.DEVIATION 0.10756

PERCENTILES: 2.5%1.500E-02 5.0%2.346E-02 50.0% .104 95.0% .360 97.5% .416

500 POINT HISTOGRAM * = 1 POINTS

PROB	CUME	VALUE		
0.0320	0.0000	0.0000E+00	16	**********
0.1040	0.0320	2.0000E-02	52	**********
0.1240	0.1360	4.0000E-02	62	**********
0.1220	0.2600	6.0000E-02	61	**********
0.0980	0.3820	8.0000E-02	49	**********
0.0960	0.4800	0.1000	48	**********
0.0780	0.5760	0.1200	39	**********
0.0480	0.6540	0.1400	24	**********
0.0400	0.7020	0.1600	20	**********
0.0300	0.7420	0.1800	15	**********
0.0340	0.7720	0.2000	17	**********
0.0380	0.8060	0.2200	19	********** (BL)
0.0280	0.8440	0.2400	14	**********
0.0220	0.8720	0.2600	11	**********
0.0180	0.8940	0.2800	9	**********
0.0120	0.9120	0.3000	6	******
0.0140	0.9240	0.3200	7	*******
0.0120	0.9380	0.3400	6	******
0.0100	0.9500	0.3600	5	*****
0.0060	0.9600	0.3800	3	***
0.0100	0.9660	0.4000	5	*****
0.0040	0.9760	0.4200	2	**
0.0060	0.9800	0.4400	3	***
0.0020	0.9860	0.4600	1	*
0.0000	0.9880	0.4800	0	
0.0040	0.9880	0.5000	2	**
0.0020	0.9920	0.5200	1	*
0.0020	0.9940	0.5400	1	*
0.0020	0.9960	0.5600	1	*
0.0000	0.9980	0.5800	0	
0.0020	0.9980	0.6000	1	*
	1.0000	0.6200		

Baseline Value (BL)
0.2

Figure I.18 (Continued)

STATISTICS FOR OUTPUT VARIABLE CPHOT (Cost per Mole of UV Photons, $/Einstein)

MINIMUM 2.2839 MAXIMUM 5.5729

MEAN 3.6062 VARIANCE 0.23336 STD.DEVIATION 0.48308

PERCENTILES: 2.5% 2.69 5.0% 2.86 50.0% 3.57 95.0% 4.44 97.5% 4.55

500 POINT HISTOGRAM * = 1 POINTS

PROB	CUME	VALUE		
0.0020	0.0000	2.200	1	*
0.0000	0.0020	2.300	0	
0.0060	0.0020	2.400	3	***
0.0020	0.0080	2.500	1	*
0.0160	0.0100	2.600	8	********
0.0100	0.0260	2.700	5	*****
0.0240	0.0360	2.800	12	************
0.0420	0.0600	2.900	21	**********************
0.0500	0.1020	3.000	25	*************************
0.0420	0.1520	3.100	21	**********************
0.0740	0.1940	3.200	37	*************************************
0.0700	0.2680	3.300	35	***********************************
0.0940	0.3380	3.400	47	***
0.0940	0.4320	3.500	47	***
0.0600	0.5260	3.600	30	******************************
0.0740	0.5860	3.700	37	*************************************
0.0760	0.6600	3.800	38	**************************************
0.0580	0.7360	3.900	29	****************************
0.0460	0.7940	4.000	23	**********************
0.0460	0.8400	4.100	23	**********************
0.0320	0.8860	4.200	16	****************
0.0200	0.9180	4.300	10	********** ← (BL)
0.0300	0.9380	4.400	15	***************
0.0120	0.9680	4.500	6	******
0.0060	0.9800	4.600	3	***
0.0020	0.9860	4.700	1	*
0.0060	0.9880	4.800	3	***
0.0040	0.9940	4.900	2	**
0.0000	0.9980	5.000	0	
0.0000	0.9980	5.100	0	
0.0000	0.9980	5.200	0	
0.0000	0.9980	5.300	0	
0.0000	0.9980	5.400	0	
0.0020	0.9980	5.500	1	*
	1.0000	5.600		

Baseline Value

$4.4/Einstein

$/Einstein

Figure I.18 (Continued)

STATISTICS FOR OUTPUT VARIABLE WATTAV (Laser System Output Power in Watts)

MINIMUM 8824.7 MAXIMUM 6.64208E+05

MEAN 79686. VARIANCE 7.03495E+09 STD.DEVIATION 83875.

PERCENTILES: 2.5%1.161E+04 5.0%1.393E+04 50.0%5.250E+04 95.0%2.450E+05 97.5%3.000E+05

500 POINT HISTOGRAM * = 1 POINTS

PROB	CUME	VALUE		
0.0060	0.0000	0.0000E+00	3	***
0.1120	0.0060	1.0000E+04	56	**********
0.1380	0.1180	2.0000E+04	69	**********
0.1060	0.2560	3.0000E+04	53	**********
0.1220	0.3620	4.0000E+04	61	********** (BL)
0.0640	0.4840	5.0000E+04	32	**********
0.0860	0.5480	6.0000E+04	43	**********
0.0560	0.6340	7.0000E+04	28	**********
0.0420	0.6900	8.0000E+04	21	**********
0.0280	0.7320	9.0000E+04	14	**********
0.0280	0.7600	1.0000E+05	14	**********
0.0340	0.7880	1.1000E+05	17	**********
0.0240	0.8220	1.2000E+05	12	**********
0.0220	0.8460	1.3000E+05	11	**********
0.0080	0.8680	1.4000E+05	4	****
0.0200	0.8760	1.5000E+05	10	**********
0.0060	0.8960	1.6000E+05	3	***
0.0060	0.9020	1.7000E+05	3	***
0.0040	0.9080	1.8000E+05	2	**
0.0140	0.9120	1.9000E+05	7	*******
0.0060	0.9260	2.0000E+05	3	***
0.0060	0.9320	2.1000E+05	3	***
0.0020	0.9380	2.2000E+05	1	*
0.0040	0.9400	2.3000E+05	2	**
0.0120	0.9440	2.4000E+05	6	******
0.0040	0.9560	2.5000E+05	2	**
0.0020	0.9600	2.6000E+05	1	*
0.0040	0.9620	2.7000E+05	2	**
0.0060	0.9660	2.8000E+05	3	***
0.0020	0.9720	2.9000E+05	1	*
0.0040	0.9740	3.0000E+05	2	**
0.0000	0.9780	3.1000E+05	0	
0.0020	0.9780	3.2000E+05	1	*
0.0020	0.9800	3.3000E+05	1	*
0.0000	0.9820	3.4000E+05	0	
0.0000	0.9820	3.5000E+05	0	
0.0000	0.9820	3.6000E+05	0	
0.0000	0.9820	3.7000E+05	0	
0.0000	0.9820	3.8000E+05	0	
0.0020	0.9820	3.9000E+05	1	*
	0.9840	4.0000E+05		

Watts

(BL) Baseline (BL)
27,230 Watts

Figure I.18 (Continued)

STATISTICS FOR OUTPUT VARIABLE CTOT (Syngas Cleanup System Capital Cost)

MINIMUM 3.14739E+07 MAXIMUM 9.74994E+08

MEAN 1.31754E+08 VARIANCE 1.27877E+16 STD.DEVIATION 1.13083E+08

PERCENTILES: 2.5%4.000E+07 5.0%4.260E+07 50.0%9.550E+07 95.0%3.400E+08 97.5%4.200E+08

500 POINT HISTOGRAM * = 2 POINTS

PROB	CUME	VALUE		
0.0240	0.0000	2.0000E+07	12	******
0.2000	0.0240	4.0000E+07	100	** ← (BL)
0.1520	0.2240	6.0000E+07	76	**************************************
0.1600	0.3760	8.0000E+07	80	**
0.0780	0.5360	1.0000E+08	39	********************
0.0860	0.6140	1.2000E+08	43	**********************
0.0660	0.7000	1.4000E+08	33	*****************
0.0480	0.7660	1.6000E+08	24	************
0.0320	0.8140	1.8000E+08	16	********
0.0200	0.8460	2.0000E+08	10	*****
0.0240	0.8660	2.2000E+08	12	******
0.0180	0.8900	2.4000E+08	9	*****
0.0120	0.9080	2.6000E+08	6	***
0.0120	0.9200	2.8000E+08	6	***
0.0060	0.9320	3.0000E+08	3	**
0.0120	0.9380	3.2000E+08	6	***
0.0080	0.9500	3.4000E+08	4	**
0.0040	0.9580	3.6000E+08	2	*
0.0020	0.9620	3.8000E+08	1	*
0.0100	0.9640	4.0000E+08	5	***
0.0020	0.9740	4.2000E+08	1	*
0.0040	0.9760	4.4000E+08	2	*
0.0040	0.9800	4.6000E+08	2	*
0.0000	0.9840	4.8000E+08	0	
0.0020	0.9840	5.0000E+08	1	*
0.0020	0.9860	5.2000E+08	1	*
0.0000	0.9880	5.4000E+08	0	
0.0000	0.9880	5.6000E+08	0	
0.0000	0.9880	5.8000E+08	0	
0.0000	0.9880	6.0000E+08	0	
0.0020	0.9880	6.2000E+08	1	*
0.0020	0.9900	6.4000E+08	1	*
0.0000	0.9920	6.6000E+08	0	
0.0000	0.9920	6.8000E+08	0	
0.0020	0.9920	7.0000E+08	1	*
	0.9940	7.2000E+08		

$

Baseline Value (BL)
$57.1 Million

Figure I.18 (Continued)

STATISTICS FOR OUTPUT VARIABLE PERCT (Percent that Photolytic Syngas Cleanup System Adds to Methanol Unit Cost)

MINIMUM 8.2909 MAXIMUM 181.21

MEAN 28.847 VARIANCE 501.85 STD.DEVIATION 22.402

PERCENTILES: 2.5% 10.2 5.0% 10.8 50.0% 21.8 95.0% 72.1 97.5% 92.5

500 POINT HISTOGRAM * = 2 POINTS

PROB	CUME	VALUE		
0.0140	0.0000	5.000	7	****
0.2320	0.0140	10.00	116	**********
0.2040	0.2460	15.00	102	**********
0.1360	0.4500	20.00	68	**********
0.1140	0.5860	25.00	57	**********
0.0700	0.7000	30.00	35	**********
0.0560	0.7700	35.00	28	**********
0.0320	0.8260	40.00	16	********
0.0320	0.8580	45.00	16	********
0.0120	0.8900	50.00	6	***
0.0220	0.9020	55.00	11	******
0.0100	0.9240	60.00	5	***
0.0100	0.9340	65.00	5	***
0.0140	0.9440	70.00	7	****
0.0040	0.9580	75.00	2	*
0.0100	0.9620	80.00	5	***
0.0000	0.9720	85.00	0	
0.0040	0.9720	90.00	2	*
0.0060	0.9760	95.00	3	**
0.0020	0.9820	100.0	1	*
0.0000	0.9840	105.0	0	
0.0000	0.9840	110.0	0	
0.0020	0.9840	115.0	1	*
0.0000	0.9860	120.0	0	
0.0060	0.9860	125.0	3	**
0.0020	0.9920	130.0	1	*
0.0000	0.9940	135.0	0	
0.0000	0.9940	140.0	0	
0.0020	0.9940	145.0	1	*
0.0000	0.9960	150.0	0	
0.0000	0.9960	155.0	0	
0.0000	0.9960	160.0	0	
0.0000	0.9960	165.0	0	
0.0000	0.9960	170.0	0	
0.0020	0.9960	175.0	1	*
0.0020	0.9980	180.0	1	*
	1.0000	185.0		

(BL)

Baseline Value (BL)

14.0%

%

Figure I.18 (Continued)

Table I.17

Uncertainty Analysis Results
Including Conditional MVSS's

MVSS No.	MVSS Description	Output Statistics† Minimum	5 Percentile	Median	95 Percentile	Maximum	Mean	Standard Deviation	Mode (bin with most cases)
	Total MVSS								
1.	12 uncertainty input variables only; no MVSS or figure-or-merit adjustment factors	190.7	196	215	306	495	227	39.5	195 - 200
2.	14 uncertainty input variables including F_{PD} and capital cost growth factor F_{CCG}	191.4	201	227	345	612	243.9	53.5	200 - 210
	Conditional MVSS								
3.	7 performance related input variables only, 5 cost variables constant at input mode values; no figure-of-merit adjustment factors	191.3	196	213	295	470	224.2	38.3	195 - 200
4.	5 cost related input variables only, 7 performance variables held constant at mode values; no figure-of-merit adjustment factors	199.7	201	206	209	212	205.6	2.25	206.0 - 206.5

†Figure of Merit: Unit Methanol Production Cost.

standard deviation (σ) (from the twelve variable MVSS (No. 1) should be noted.

From the results above, one would conclude that the developer projected a optimistic baseline. This tendency is very common in early economic evaluations and is part of the purpose for development of this methodology. Up to this point the uncertainty analysis has been considered only in relation to the baseline for the same process. It is now of interest to compare the projected photolytic syngas cleanup costs to those for other more conventional proposed sulfur removal techniques.

Comparison With Other Sulfur Removal Methods

The conventional method of removing sulfur from synthesis gas is adsorption on a zinc oxide (ZnO) catalyst guard bed at approximately 350°C (660°F). In the article by R. Dalla Betta and K. Ushiba[123] and the EPRI report[124] the economics of the baseline methanol production plant are discussed for both ZnO sulfur removal and the alternative of developing a sulfur tolerant methanol synthesis catalyst which can operate at 5 to 100 ppm H_2S without rapid degradation. The contribution of the methanol synthesis plant and sulfur removal equipment to the unit cost of methanol can be separated and the following results obtained. For the baseline methanol plant alone, the total unit production costs contribute $23.4 per ton of methanol. (For all cases here discussed the syngas unit feedstock costs and Claus plant unit costs account for $145.4 and $7.3 per ton, respectively.) With no sulfur removal an alcohol cost of $176.1 per ton results. Addition of a ZnO desulfurization system adds $2 per ton of methanol to the total cost to obtain a total cost of $178.1 per ton. It should be noted that the methanol plant and

ZnO desulfurization costs used from the article referenced were escalated before use to conform with the same year (1982) as the photolysis process.

It is readily apparent that even the most optimistic (minimum) methanol unit cost of $191/ton from the photolytic process uncertainty histogram (Fig. 9.9) is $13 per ton above the total methanol cost including ZnO desulfurization derived from the literature. This result is in contrast to the rough projection in the paper by Chen and Borzileri[125] which projected a possible 1% or $1.60 per ton increase in the cost of methanol (in their case a methanol unit cost of $158 per ton or $175 per metric ton cost was used).

Performance was not assumed to be an issue for the ZnO conventional process. Any uncertainty would be small compared to the laser photolysis process uncertainty envelope. This difference is due to the fact that a conventional process (probably RD&D Level IV or V) for which costs are well known is being compared to a process for which an economic estimate was based on very incomplete design and cost calculations (RD&D Level I). The photolytic desulfurization process also has never had the benefit of even benchscale determination of its performance potential. To the author's best knowledge, the theoretical and economic analysis presented here is the most detailed and complete study on photolytic desulfurization written to date. The question might be raised as to why the preliminary estimate in Chen and Borzileri's paper[126] projected such low costs. Most of the difference manifested itself as the process was modeled and analyzed as the basis for this study. The next subsection lists the major contributors to increased cost projections.

Observations and Conclusions

Explanations for the Appearance of Less Favorable Than Projected Economics of the Photolytic Syngas Cleanup Process in This Analysis

1. The initial calculation (Chen and Borzileri) did not include the considerable costs of gas handling necessitated by the differences in the pressures at which the photolysis and the other syngas handling and methanol synthesis steps operate. Recompression of the clean syngas prior to methanol synthesis is a major operating cost. The gas handling and its associated thermodynamic implication require the use of much additional energy management equipment, which further increases capital and operating costs.

2. The initial estimate did not include balance-of-plant items, a building, or the costs associated with sulfur collection. Only laser system capital and operating costs were considered.

3. The photolytic process might be economic only for removal of very trace amounts of sulfur, i.e., down to levels of tens of parts per billion or less which cannot be accomplished via conventional chemical separation techniques. It is doubtful that there is significant demand for methanol of such high purity and if there were, methanol synthesis feedstocks other than coal-derived syngas could be used.

Conditional MVSS Observations

Table I.17 shows two additional MVSS's (Nos. 3 & 4) in which seven performance and five cost related uncertainty inputs were separately examined. These two MVSS cases (histogram Fig. 10.1) were discussed in detail in Chapter X and support the first main conclusion drawn from this study.

APPENDIX J

FORTRAN ASSESSMENT MODEL FOR PHOTOLYTIC SYNGAS CLEANUP PROCESS

CONTROL ROUTINE, PHOTOLYSIS CALCULATIONS, LASER POWER REQ'TS, COLLECTOR DESIGN, AND REOPTIMIZATION SCHEME

```
      SUBROUTINE FUNCT
      REAL MGAS,MH2S,NH2S,NGAS,MOLSEC,MS,MOSULF,LBSULF,KGSULF,LAMBDA,K,
     1MOPHOT,LSYN,LHS,MHS,MFSULF,NFOLD,MH2,MCO,MOFLOW,MOCLN,KGCLN,MGASF,
     2MGASP,LBMS,MACHMX,MOSULB,MOFLWB,NGASC,NH2SC,KW,KWPUMP,KWREFR,
     3KWEQUI,KWTOT,KWHR,KWNET,KWUSE,KWCAPB,KWCAP,MWN
      COMMON /WHY/FDRQKG,SIGMA,TEMP,TORR,PPMH2S,FRMCH,HIZ,WIZ,
     1PCOLLF,COLLIF,RECRAT,COUNIT,CCPWAT,OCPWAT,EFF,FPD,FCOG,FOOG,FPDF,
     2PUTIL,PHIUV,MWN,WATTAV,AVAIL,CGH,CLRCC,CTOT,
     3ANCOST,CPHOT,COGH,CUNIT,STAFF,PERCT,COSTT,PATHL,
     4TON,Y(9)
      COMMON /PRINT/ ITER,INTER,IPR
      DIMENSION A(3)
      DATA LAMBDA/210./,SIGCO/8.E-24/,NFOLD/0./
      DATA PPMCLN/.1/,OPTREP/0.5/,COLREP/0.25/
      DATA A/'F   ','P   ','W(S)'/
      IF(ITER.LE.IPR)
     *WRITE(6,666)FDRQKG,SIGMA,TEMP,TORR,PPMH2S,FRMCH,HIZ,WIZ,
     1PCOLLF,COLLIF,RECRAT,COUNIT,CCPWAT,OCPWAT,EFF,FPD,FCOG,FOOG,FPDF
  666 FORMAT('1FDRQKG=',T30,E9.3,/,' SIGMA=',T30,E9.3,/,' TEMP=',T30,
     1F9.1,/,' TORR=',T30,F9.1,/,' PPMH2S=',T30,F9.1,/,' FRMACH=',
     2T30,F9.2,/,' HIZ=',T30,F9.2,/,' WIZ=',T30,F9.2,/,' PCOLLF=',T30,
     3F9.1,/,' COLLIF=',T30,F9.1,/,' RECRAT=',T30,E9.2,/,' COUNIT=',
     4T30,F9.0,/,' CCPWAT=',T30,F9.0,/,' OCPWAT=',T30,F9.0,/,' EFF=',
     5T30,F9.4,/,' FPD=',T30,F9.3,/,' FCOG=',T30,F9.3,/,' FOOG='
     6,T30,F9.3,/,' FPDF=',T30,F9.3,///)
C     PHYSICAL CONSTANTS
      C=3.E10
      H=6.625E-34
      EVJ=6.24E18
C   ESTIMATE OF OPTICS LIFETIME FROM FLUENCE ESTIMATE
      EP=H*C/(LAMBDA*1.E-7)
      FLUEST=EP*(-ALOG(1.-0.99))/SIGMA
      OPTLIF=25./FLUEST
C   CALCULATION OF PLANT AVAILABILITY
C   CALL RAM SUBROUTINE
      CALL RAM(OPTLIF,OPTREP,COLLIF,COLREP,AVAIL)
C   DESIGN FEEDRATE DEPENDS ON PLANT AVAILABILITY
      FEEDKG=FDRQKG/AVAIL
C   BASE CASE VALUES FOR COST SCALING
      POWHDB=1238.
```

```
      WTURBB=16970.
      WCOMPB=37940.
      MOSULB=2.975E5
      MOFLWB=1.3375E8
      NHEADB=22
      KWCAPB=6851.
      AVAILB=0.93291
      ATOTB=16500.
C     PRESSURE IN COAL GASIFIER
      PCOAL=31.6*760.
      TCOALK=322.
C     PRESSURE IN SYNGAS CATALYSIS UNIT
      PSYN=76.*760.
      TSYNF=448.
C     TEMPORARY PUMP DATA
C    CONSTANTS
      RH2CO=2.
      MH2=2.
      MCO=28.
      PI=3.1416
      AVO=6.02380E23
      MGAS=(RH2CO/(RH2CO+1.))*MH2+(1.-(RH2CO/(RH2CO+1.)))*MCO
      MGASF=(PPMH2S/1.E6)*MH2S+(1.-PPMH2S/1.E6)*MGAS
      GMOLE=22414.0
      SECYR=3.154E7
      MS=32.
      MH2S=34.
C    GAS CONSTANTS FOR VARYING UNITS
      RGAS=1.0354E-19
      RGAS1=1546.
      GRAV=32.17
      CPRAT=1.406
      MACHMX=SQRT(2.)/SQRT(CPRAT-1.)
C     INPUTS:
    7 FORMAT(1H1)
      IF(ITER.LE.IPR)
     1WRITE(6,16)
   16 FORMAT(' ',///)
C     CALCULATIONS
C     FEED CALC.
      FRMACH=FRMCH
      FEEDLB=FEEDKG*2.205
C    VOLUMETRIC FLOW OF SYNGAS
      CM3SC=(FEEDKG*1000./MGASF)*(GMOLE/SECYR)*(TEMP/273.)*(760./TORR)
      SCF=(FEEDKG*1000./MGASF)*(GMOLE/1000.)*0.03531
      SCFM=SCF/(365.*24.*60.)
      MOFLOW=(SCF/359.05)
C    SYNGAS NUMBER DENSITY
      NGAS=TORR/(RGAS*TEMP)
C    H2S NUMBER DENSITY
```

```
      NH2S=(PPMH2S/1.E6)*NGAS
C     H2S PARTIAL PRESSURE
      PPH2S=(PPMH2S/1.E6)*TORR
      XF=(PPMH2S/1.E6)*(MS/MGASF)
      XXF=(PPMH2S/1.E6)
C     MOLES OF H2S PASSING IRR ZONE PER SEC
      MOLSEC=(FEEDKG*1000./SECYR)*(PPMH2S/1.E6)*(1./MGAS)*AVO
      MFSULF=MOLSEC/AVO*SECYR
C     CALC OF SYNGAS SONIC VELOCITY
      VSONIC=30.48*SQRT((GRAV*CPRAT*RGAS1*TEMP*1.8)/MGAS)
      VEL=FRMACH*VSONIC
C     MAXIMUM EXPANSION VELOCITY TO VACUUM
      VMAX=VSONIC*SQRT(2.)/SQRT(CPRAT-1.)
C     CRITICAL PRESSURE RATIO
      CPR=(2./(CPRAT+1.))**(CPRAT/(CPRAT-1.))
C     CRITICAL TEMPERATURE RATIO
      CTR=2./(CPRAT+1.)
C     CALC OF THROAT HEIGHT RATIO AS A FCN. OF MACH # IN EXPANSION ZONE
      TERM1=1.+((CPRAT-1.)/2.)*FRMACH**2.
      TERM2=(2./(CPRAT+1.))*TERM1
      HRAT=1./(SQRT((1./FRMACH**2.)*(TERM2**((CPRAT+1.)/(CPRAT-1.)))))
      HNOZ=HRAT*HIZ
C     CALC OF PRESSURE RATIO IN EXP ZONE TO THAT IN FRONT OF NOZZLE THRT.
      CALL PRATIO(HRAT,CPR,CPRAT,PRAT)
      P0=TORR/PRAT
C     PRESSURE AT THROAT
      PT=P0*CPR
C     PRE-EXPANSION TEMP NEEDED TO GET DESIRED IRR ZONE TEMP
      T0=TEMP/((PRAT)**((CPRAT-1.)/CPRAT))
C     THROAT TEMP
      TT=T0*CTR
C     REQUIRED NOZZLE FLOW AREA(WNOZ*HIZ*NFOLD)
      AFLOW=CM3SC/VEL
      ANOZ=HRAT*AFLOW
C     NOZZLE LENGTH CALC( WNOZ IS (1/NFOLD)*THE  LASER BEAM PATH LENGTH)
      WNOZ=AFLOW/(HIZ*(NFOLD+1.))
C     GAS TRANSIT TIME THROUGH IRRADIATION ZONE
      TRANST=WIZ/VEL
C     IRR ZONE X-SECT AREA (ALSO X-SECT AREA OF LASER BEAM)
      XCBEAM=WIZ*HIZ
C     DIFFRACTION LIMITING PATH LENGTH &FRESNEL NUMBER
      WAVE=LAMBDA*1.E-7
      ASPECT=WIZ/HIZ
      IF(ASPECT.GE.1) ZIZ=HIZ
      IF(ASPECT.LT.1) ZIZ=WIZ
      FRESNL=(ZIZ**2)/(WNOZ*WAVE)
      DIFFL=(ZIZ**2)/(0.8*WAVE)
C     IRRADIATION ZONE VOLUME
      PATHL=WNOZ*(NFOLD+1.)
      VOLIZ=XCBEAM*WNOZ*(NFOLD+1.)
```

```
      IF(ITER.LE.IPR)
     1WRITE(6,11)FEEDLB,FEEDKG,CM3SC,NGAS,TEMP,TORR,VSONIC,FRMACH,VEL,
     1SCF,MGASF,RH2CO
   11 FORMAT('   SYNGAS DATA:',/,'     FEEDLB= ',1PE11.3,' LB/YR
     1FEEDKG= ',1PE11.3,' KG/YR',/,'     VOLUMETRIC FLOWRATE
     2(CM3SC)= ',1PE11.3,' CM3/SEC      AT A DENSITY OF',/,5X,1PE11.3,
     3' MOLECULES/CM3',/,'     TEMP= ',0PF5.0,' K      PRESSURE= ',
     40PF5.0,' TORR      SONIC VELOCITY= ',0PF7.0,' CM/SEC',/,
     5'     GAS VELOCITY IS ',0PF8.4,' OF SONIC OR ',0PF10.3,'CM/SEC',
     66X,'VOLUME FLOW IS  ',1PE11.3,' SCF/YR',/
     7,5X,'AVE SYNGAS MOL.WT. = ',0PF8.3,6X,'H2 TO CO RATIO IN FEED=
     8 ',0PF5.1,//)
C    COLLECTOR PRESSURE IS 0.1 TO 1.2 TIMES THE INT ZONE PRESSURE
      PCOLL=PCOLLF*TORR
C
      CALL TURBIN(PCOAL,TCOALK,P0,T0,MOFLOW,MGAS,WTOT,QTOT,HPTOT,TTO1)
      CALL COMPRS(SCF,PCOLL,PSYN,MOFLOW,MGAS,HPNT,COSTT,QT,QAVAIL,TEND,
     1NCOMP)
      WTURB=HPTOT
      WCOMP=HPNT
      CALL ENERGY(WTURB,WCOMP,TEND,QAVAIL,QT,QTOT,TTO1,TSYNF,MGAS,
     1MOFLOW,SREQCP,SREQME,KWHR,ATURB,ACOMP,AMEX,TONS,GPM,KWPUMP,KWREFR,
     2SREQ,KWEQUI,KW)
      IF(ITER.LE.IPR)
     1WRITE(6,810) VMAX,VSONIC,VEL
      IF(ITER.LE.IPR)
     1WRITE(6,820) P0,T0,PSYN
      IF(ITER.LE.IPR)
     1WRITE(6,830) HIZ,PT,WIZ,CPR,FRMACH,PCOLL,TT,TEMP,TORR
      IF(ITER.LE.IPR)
     1WRITE(6,840) WNOZ,AFLOW,ANOZ,WCOMP
      IF(ITER.LE.IPR)
     1WRITE(6,850)
      IF(ITER.LE.IPR)
     1WRITE(6,860) WTURB
      IF(ITER.LE.IPR)
     1WRITE(6,870) PCOAL
      IF(ITER.LE.IPR)
     1WRITE(6,21)HIZ,WIZ,XCBEAM,AFLOW,WNOZ,VOLIZ,TRANST,PATHL,FRESNL,
     1DIFFL
   21 FORMAT('   IRRADIATION ZONE DATA:',/'     IRRADIATION ZONE HT= '
     1,F6.3,' CM      IRRADIATION ZONE WIDTH= ',F6.3,' CM'/'      IRR ZN
     2 XSECT AREA= ',F9.4,' CM2',/,'     FLOW AREA THROUGH IRR ZONE= '
     3,F9.3,' CM2      NOZZLE LENGTH= ',F7.1,' CM',/,'     IRR ZONE VOL
     4 =',F9.2,' CM3'/'      TRANSIT TIME PAST IRRAD.ZONE WIDTH= ',F7.5,
     5' SEC',6X,'LASER BEAM PATH LENGTH THRU GAS= ',F7.1,' CM',/,
     6'     LASER BEAM FRESNEL NUMBER = ',F6.2,'   DIFFRACTION LIMITED
     7',/,'     PATH LENGTH(FRESNEL # OF 0.8) = ',F8.1,//)
C    MIRROR REFLECTIVITY
      REFL=0.985
C    ENERGY PER PHOTON
```

```
      EPHOT=H*C/WAVE
      EVPHOT=EPHOT*EVJ
      PULSE=1.E-7
C   REQUIRED LASER REP RATE
      REP=1./TRANST
C   MAXIMUM REP RATE FOR A LASER HEAD
      REPMAX=1250.
C   MAXIMUM OUTPUT POWER FOR A LASER HEAD
      POWMAX=7500.
C     THIS SECTION CALCULATES REQD PHOTOLYTIC CUT AND LASER
C     FLUENCE TO OBTAIN REQUIRED DECONTAMINATION
C     DESIRED W IS ELEMENTAL SULFUR
      XCLDES=PPMCLN/1.E6
      MGASP=XCLDES*MH2S+(1.-XCLDES)*MGAS
      YPDES=XCLDES*(MS/MGASP)
      WDES=FEEDKG*(XF-YPDES)/(1.-YPDES)
      PDES=FEEDKG-WDES
      XW=1.
      PMDES=PDES*2.205/MGASP
      WMDES=MOFLOW*(PPMH2S/1.E6-XCLDES)
      DECOND=(FEEDKG*XF)/(YPDES*PDES)
C      CALC . OF CUT REQUIREMENTS
      THSWO=WDES/(FEEDKG*XF)
      THSVO=THSWO
      IF(ITER.LE.IPR)
     1WRITE(6,919)
  919 FORMAT(5X,'* * * MATL BALANCES FOR DESIRED SULFUR REMOVAL * * *',/
     *)
      IF(ITER.LE.IPR)
     1WRITE(6,916)THSVO,DECOND
  916 FORMAT(10X,'STAGE S CUT OF ',F9.6,' REQD FOR A DF OF ',F7.2,//)
      IF(ITER.LE.IPR)
     1WRITE(6,171)
      IF(ITER.LE.IPR)
     1WRITE(6,172)A(1),FEEDKG,XF,MOFLOW,XXF
      IF(ITER.LE.IPR)
     1WRITE(6,172)A(2),PDES,YPDES,PMDES,XCLDES
      IF(ITER.LE.IPR)
     1WRITE(6,172)A(3),WDES,XW,WMDES,XW
C      ESTIMATE POST PHOTOLYSIS QUANTUM YIELD
C     POST-PHOTOLYSIS EFFECTS
C     GAS PROPERTIES
      MHS=33.
      RGAS2=8.314E7
C    MOLECULAR COLLISION X-SECT(CM2)
      SIGSYN=3.E-8
      SIGHS=3.5E-8
C   GAS NUMBER DENSITIES IN COLLECTION REGION
      NGASC=PCOLL/(RGAS*TEMP)
      NH2SC=(PPMH2S/1.E6)*NGASC
```

```
C     LXXX DESIGNATES MEAN FREE PATH
      LSYN=1./(1.414*PI*SIGSYN**2*NGASC)
      LHS=1./(1.414*PI*SIGHS**2*NH2SC)
C     CXXX DESIGNATES MOLECULAR VELOCITIES
      CSYN=SQRT(8.*RGAS2*TEMP/(PI*MGAS))
      CHS=SQRT(8.*RGAS2*TEMP/(PI*MHS))
C     Z1XXX DESIGNATES COLLISION OF A SINGLE MOLECULE PER SEC
      Z1SYN=1.414*PI*SIGSYN**2*CSYN*NGASC
C     THE RECIPROCAL DESIGNATES THE TIME BETWEEN COLLISIONS
      SYNCOL=1./Z1SYN
C     Z2XXX DESIGNATES COLLISIONS/CM3 PER SEC
      Z2SYN=(1./1.414)*PI*CSYN*(SIGSYN*NGASC)**2
      Z1HS=1.414*PI*SIGHS**2*CHS*NH2SC
      THSCOL=1./Z1HS
      Z2HS=(1./1.414)*PI*CHS*(SIGHS*NH2SC)**2
      IF(ITER.LE.IPR)
     1WRITE(6,918)
  918 FORMAT(5X,'* * * PROCESS QUANTUM YIELD AND PHOTOLYTIC CUT
     *REQTS FOR DESIRED SULFUR REMOVAL * * *',/)
      IF(ITER.LE.IPR)
     1WRITE(6,42)
      IF(ITER.LE.IPR)
     1WRITE(6,41)SIGHS,CHS,LHS,Z1HS,Z2HS,THSCOL
C     TOTAL CUT IS APPORTIONED BETWEEN QUANTUM YIELD AFTER POST-
C     PHOTOLYSIS BACK REACTION AND PHOTOLYTIC CUT
C     MINIMUM REQD QUANTUM YIELD
      QYR=SQRT(THSVO)
C     MINIMUM REQD PHOTOLYTIC CUT
      THPHOT=SQRT(THSVO)
C     SOLVE FOR HS RESIDENCE TIME IN COLLECTOR PORE
      ETERM=(QYR-0.5)/0.5
      TRAT=-ALOG(ETERM)
C     REACTION HALF LIFE FOR 2ND ORDER REACTION
      THALF=1./(RECRAT*NH2SC)
C     TIME HS FRAG HAS TO TRAVEL BEFORE BACK REACTING
      TAURQ=TRAT*THALF
C     DISTANCE HS FRAG WILL TRAVEL IN THIS TIME DEFINES PORE SIZE
      TUBED=CHS*TAURQ
C     FLUENCE WHICH GIVES LIMITING THPHOT
      PHFLX0=(-ALOG(1.-THPHOT))/SIGMA
      PHIUV0=PHFLX0*EPHOT
      IF(ITER.LE.IPR)
     1WRITE(6,917)QYR,TAURQ,TUBED,LHS,THPHOT,PHFLX0,PHIUV0
  917 FORMAT(10X,'REQD QUANTUM YIELD TO GET DESIRED CUT',T50,F9.6,/,
     *10X,'REQD TRANSIT TIME(SEC) TO COLLECTOR PORE WALL',T50,E9.3,/,
     *10X,'REQD PORE DIAMETER TO CAPTURE HS (CM)',T50,F9.4,/,
     *10X,'EST COLLISIONAL MEAN FREE PATH OF HS FRAG(CM)',T50,F9.4,/,
     *10X,'EST REQD PHOTOLYTIC CUT',T50,F9.6,/,
     *10X,'EST PHOTON FLUX REQD(PHOTONS/CM2-SEC)',T50,E9.3,/,
     *10X,'EST LASER FLUENCE REQD(J/CM2)',T50,F9.3,//)
      IF(ITER.LE.IPR)
```

```
      1WRITE(6,175) PPMH2S,PPMCLN,THSWO,THSVO,QYR,THPHOT,PHIUVU
  175 FORMAT('0   REQTS TO REDUCE S CONC FROM ',F5.1,' PPM  TO  ',
     1F5.1,' PPM',/,
     2'   STAGE S CUT (BY WEIGHT) = ',F10.6,/
     3'   STAGE S CUT (BY MOLAR VOL.) = ',F10.6,/
     4'   QUANTUM YIELD EST FOR POST PHOTOLYSIS EFFECTS = ',F10.4,/
     5'   REQD SULFUR PHOTOLYTIC CUT = ',F10.6,/
     6'   REQD LASER FLUENCE TO REACH ABOVE AS LIMITING CUT= ',F6.2,//)
C     PHOTON FLUX CALCULATED FORM FLUENCE
      PHIUV=PHIUV0
      ITERA=1
  100 CONTINUE
      PHFLUX=PHIUV/EPHOT
C   LASER BEAM INTENSITY(INSTANTANEOUS)
      WATTI=(PHIUV/PULSE)*XCBEAM
C     LASER BEAM INSTANTANEOUS ENERGY PER PULSE
      ENER=PHIUV*XCBEAM
C   AVERAGE LASER OUTPUT POWER
      WATTAV=PHIUV*REP*XCBEAM
C    MOLES OF PHOTONS GENERATED PER YEAR
      MOPHOT=(WATTAV/EPHOT)*SECYR/AVO
C   LASER WALLPLUG POWER
      WALLPG=WATTAV/EFF
      TERM=EXP(SIGMA*PHFLUX)-1.
C    LIMITING PHOTOLYTIC CUT FOR THE GIVEN FLUENCE
      THLIM=1.-EXP(-SIGMA*PHFLUX)
C   PHOTOLYTIC CUT AT WNOZ
      THETA=(EXP(-SIGMA*NH2S*PATHL)*TERM)/(1.+(EXP(-SIGMA*NH2S*PATHL)
     1*TERM))
      K=SIGMA*NH2S
C    ABSORBTION OF UV BY H2S
      ENSIGW=NH2S*SIGMA*PATHL
C    ABSORBTION OF UV BY CO IN SYNGAS
      ENSWCO=NGAS*SIGCO*PATHL
C    ABSORBTION RATIO
      ABSRAT=ENSIGW/ENSWCO
C    INTEGRAL OF PHOTO CUT FOR 0 TO PATHL
      THINT=(-1/K)*ALOG((1.+EXP(-K*PATHL)*(EXP(SIGMA*PHFLUX)-1.))/
     1EXP(SIGMA*PHFLUX))
C    AVERAGE PHOTOLYTIC CUT OVER ENTIRE IRRAD.ZONE
      THAVE=(THINT/PATHL)*REFL**(2.*NFOLD)
C    PHOTON UTILIZATION
      PUTIL=NH2S*PATHL*THAVE/PHFLUX
C     POST-PHOTOLYSIS EFFECTS
C     GAS PROPERTIES
      MHS=33.
      RGAS2=8.314E7
C    MOLECULAR COLLISION X-SECT(CM2)
      SIGSYN=3.E-8
      SIGHS=3.5E-8
```

```
C     LXXX DESIGNATES MEAN FREE PATH
      LSYN=1./(1.414*PI*SIGSYN**2*NGASC)
      LHS=1./(1.414*PI*SIGHS**2*NH2SC*THAVE)
C     CXXX DESIGNATES MOLECULAR VELOCITIES
      CSYN=SQRT(8.*RGAS2*TEMP/(PI*MGAS))
      CHS=SQRT(8.*RGAS2*TEMP/(PI*MHS))
C     Z1XXX DESIGNATES COLLISION OF A SINGLE MOLECULE PER SEC
      Z1SYN=1.414*PI*SIGSYN**2*CSYN*NGASC
C     THE RECIPROCAL DESIGNATES THE TIME BETWEEN COLLISIONS
      SYNCOL=1./Z1SYN
C     Z2XXX DESIGNATES COLLISIONS/CM3 PER SEC
      Z2SYN=(1./1.414)*PI*CSYN*(SIGSYN*NGASC)**2
      Z1HS=1.414*PI*SIGHS**2*CHS*NH2SC*THAVE
      THSCOL=1./Z1HS
      Z2HS=(1./1.414)*PI*CHS*(SIGHS*NH2SC*THAVE)**2
C     METAL COLLECTOR TUBE DIAMETER
C     TIME REQD FOR AVERAGE HS FRAG. TO HIT COLLECTOR WALL
      TWALL=TUBED/CHS
C     TAU IS THE TRANSIT TIME FOR AN AVE.MOLECULE TO REACH
C      THE WALL,EVEN IF A FEW COLLISIONS ARE ENCOUNTERED
      TAU=TWALL
C     REACTION HALF LIFE FOR 2ND ORDER REACTION
      THALF=1./(RECRAT*NH2SC*THAVE)
C     CALC OF QUANTUM YIELD
      QY=0.5+0.5*(EXP(-TAU/THALF))
      THSTG=QY*THAVE
      IF(THSTG.LT.THSVO) PHIUV=PHIUV+0.01
      IF(THSTG.GE.THSVO) GO TO 101
      ITERA=ITERA+1
  801 FORMAT(5X,'ITERA= ',I2,
     1'   THSTG=',F13.8,'  QY=',F13.8,'  THAVE=',F13.8,
     2/)
      IF(ITERA.LE.50) GO TO 800
      IF(ITER.LE.IPR)
     1WRITE(6,821)
  821 FORMAT(5X,'FAILED AFTER 50 ITERATIONS',/)
      GO TO 300
  800 CONTINUE
      IF(ITER.LE.IPR)
     1WRITE(6,801)ITERA,THSTG,QY,THAVE
      GO TO 100
C     TOTAL MOLES OF SULFUR REMOVED
  101 MOSULF=QY*MOLSEC/AVO*SECYR*THAVE
      KGSULF=MOSULF*MS/1000.
      MOCLN=MOFLOW-MOSULF
      KGCLN=FEEDKG-KGSULF
      LBSULF=KGSULF*2.205
      LBMS=LBSULF/MS
      CLEAN=((MFSULF*MS/1000.-KGSULF)/(FEEDKG-KGSULF))*1.E6*(MGASP/MS)
      XCLN=CLEAN/1.E6
```

```
      YP=XCLN*(MS/MGASP)
C     TOTAL STAGE CUT
      SCUT=MOSULF/MFSULF
      IF(ITER.LE.IPR)
     1WRITE(6,829)
  829 FORMAT(5X,'* * * ACTUAL POST-PHOTOLYSIS MATERIAL BALANCES * * *',/
     *)
      IF(ITER.LE.IPR)
     1WRITE(6,801)ITERA,THSTG,QY,THAVE
      IF(ITER.LE.IPR)
     1WRITE(6,12) PPMH2S,NH2S,MOLSEC,MOSULF,KGSULF,LBSULF,PPH2S,MFSULF,
     1CLEAN
   12 FORMAT('   H2S DATA:',/,'     H2S CONC. IN SYNGAS= ',F4.0,
     1' PPM      NUMBER DENSITY= ',1PE11.3,' MOLECULES/CM3',/,
     2'    MOLECULES H2S/SEC= ',1PE11.3,'     G-MOLES OF S REMOVED/YR= '
     3,0PF11.2,/,
     4'     KG S REMOVED= ',0PF10.2,'      LB S REMOVED/YR= ',0PF10.2,4X,
     5'H2S PART PRESS= ',1PE11.3,' TORR'/5X,'G-MOLES OF S IN FEED/YR= '
     6,0PF11.2,5X,'PPM H2S IN CLEAN SYNGAS= ',0PF8.2,//)
      IF(ITER.LE.IPR)
     1WRITE(6,5)LAMBDA,PHFLUX,PHIUV,SIGMA,NH2S,K,ENSIGW,THLIM,THETA,
     1THAVE,WNOZ,PUTIL,PULSE,REP,EFF,WATTI,WATTAV,WALLPG,MOPHOT,ENSWCO
     2,ABSRAT,ENER
    5 FORMAT('0PHOTOLYSIS & E-O DATA:',/
     1      ,'0LAMBDA=',F6.1,'   PHFLUX =',1PE8.1,'   PHIUV=',0PF6.3,
     1'   SIGMA=',1PE8.1,/,'   NH2S=',1PE8.1,'   K=',1PE8.2,'   ENSIGW=',
     21PE8.2,/,'   THLIM=',0PE12.6,'   THETA=',0PE12.6,'   THAVE=',
     30PE12.6,'   WNOZ=',0PF7.1,/,'   PUTIL=',0PF8.5,'   PULSE=',1PE8.2,
     4'   REP=',1PE8.2,'  EFF=',1PE9.3,'  WATTI=',1PE9.3,/,'   WATTAV=',
     51PE9.3,'   WALLPG=',1PE9.2,'    MOLES OF PHOTONS/YR= ',1PE8.2,/,
     63X,'N*SIGMA*L FOR SYNGAS= ',1PE8.2,6X,'RATIO OF H2S ABS TO CO ABS=
     7 ',1PE8.2,/'   LASER PULSE ENERGY = ',0PF6.3,' JOULES',///)
      IF(ITER.LE.IPR)
     1WRITE(6,39)
   39 FORMAT('          ****POST-PHOTOLYSIS EFFECTS****',//)
      IF(ITER.LE.IPR)
     1WRITE(6,40)
   40 FORMAT('0  AVERAGE SYNTHESIS GAS COLLISIONAL DATA:'/)
      IF(ITER.LE.IPR)
     1WRITE(6,41)SIGSYN,CSYN,LSYN,Z1SYN,Z2SYN,SYNCOL
   41 FORMAT('   COLL X-SECT= ',1PE8.1,' CM2      MOLEC SPEED= ',1PE8.2,
     1'CM/SEC',/,'   MEAN FREE PATH= ',1PE10.3,' CM      COLL/SEC= ',
     21PE8.2,'      COLL/(CM3*SEC)= ',1PE8.2,6X,'TIME BETWEEN COLLISIONS
     3= ',1PE8.2,///)
      IF(ITER.LE.IPR)
     1WRITE(6,42)
   42 FORMAT('0  AVERAGE HS FRAGMENT COLLISIONAL DATA:'/)
      IF(ITER.LE.IPR)
     1WRITE(6,41) SIGHS,CHS,LHS,Z1HS,Z2HS,THSCOL
      IF(ITER.LE.IPR)
```

```
     1WRITE(6,43) RECRAT,THALF,TUBED,TAU,QY
   43 FORMAT('  HS FRAGMENT RECOMBINATION DATA:',/,'   KINETIC RATE
     1CONSTANT= ',1PE8.1,' CM3/(MOLECULE*SEC)      T 1/2 = ',1PE10.3,
     2' SEC',/,'   COLLECTOR TUBE DIAM.= ',0PF7.3,' CM      HS TRANSIT
     3 TO WALL= ',1PE8.2, ' SEC      QUANTUM YIELD= ',0PF6.3,//)
      IF(ITER.LE.IPR)
     1WRITE(6,171)
  171 FORMAT('0',T8,'KG/YR',T22,'WT.FRACT S',T35,'LB-M/YR',T48,'M/O S'
     1,/)
      IF(ITER.LE.IPR)
     1WRITE(6,172)A(1),FEEDKG,XF,MOFLOW,XXF
  172 FORMAT(' ',A4,E13.8,1X,F11.8,1X,E13.8,1X,F11.8,/)
      IF(ITER.LE.IPR)
     1WRITE(6,172)A(2),KGCLN,YP,MOCLN,XCLN
      IF(ITER.LE.IPR)
     1WRITE(6,172)A(3),KGSULF,XW,LBMS,XW
      REACTV=MOLSEC*SCUT/(VOLIZ*AVO)
      DF=(MOFLOW*XXF)/(MOCLN*XCLN)
      IF(ITER.LE.IPR)
     1WRITE(6,176) DF,REACTV
  176 FORMAT(' ',4X,'VOLUMETRIC DECONTAMINATION FACTOR:  ',F7.2,/,
     1'     REACTIVITY IN G-MOLES/CM3/SEC:    ',0PE10.4,//)
C   UNIT COST OF COLLECTOR DEPENDS ON PORE OR TUBE DIAMETER
      CLUNIT=168.8/TUBED
      IF(CLUNIT.LT.500.) CLUNIT=500.

C     CALL ECONOMICS SUBROUTINES

      CALL LASDES(REPMAX,REP,PHIUV,XCBEAM,POWMAX,POWHD,
     1POWHDB,NHEAD,NSETS,NHDSET)

      CALL LAYOUT(WNOZ,WIURB,WIURBB,WCOMP,WCOMPB,NHEAD,POWHD,
     1POWHDB,MOSULF,MOSULB,MOFLOW,MOFLWB,ATOT)

      CALL ELECTR(KW,KWPUMP,KWREFR,WALLPG,AVAIL,ATOT,POWRI,
     1POWRO,KWEQUI,KWTOT,KWUSE,KWCAP)

      CALL CAPCOS(WNOZ,WIURB,WIURBB
     1,NCOMP,POWHDB,MOSULB,MOSULF,MOFLOW,MOFLWB,CCPWAT,
     2COSTT,WATTAV,ACOMP,HPNT,ATURB,TONS,AMEX,CTOT,SCFM,P0,GPM,NHEAD,
     3NHEADB,WALLPG,ATOT,POWRI,SREQ,KWCAP,KWCAPB,CLRCC,CGH,COUNIT,
     4CLUNIT,FCOG,FPDF)

      CALL LABOR(MOFLOW,MOFLWB,OPTLIF,COLLIF,NSTAFF,AVAIL,SALTOT,
     1OPRATE,CLRATE,POWHD,POWHDB)

      CALL OPRCOS(FEEDKG,MOPHOT,WALLPG,WATTAV,SCUT,KGSULF,SCF,SREQCP,
     1SREQME,KWHR,CCPWAT,CTOT,KWUSE,POWRO,AVAIL,OPTLIF,COLLIF,NSTAFF,
     2SALTOT,OCPWAT,COUNIT,CLUNIT,KWCAPB,KWCAP,ATOT,ATOTB,MOFLOW,
     3MOFLWB,OPRATE,CLRATE,CLRCC,CGH,MFSULF,EVPHOT,MOSULF,
```

```
     4MWN,ANCOST,CPHOT,COGH,CUNIT,PERCT,TON,FPD,FCOG,FOOG,FPDF)
      STAFF=FLOAT(NSTAFF)
  300 CONTINUE
  810  FORMAT(T17,'NOZZLE CALCULATIONS',T80,'1',/,
     *T49,10('*'),T80,'2',/,
     *T25,'VMAX=',F9.1,1X,'CM/S',T48,'*',T59,'*',T80,'3',/,
     *T25,'VSONIC=',F9.1,T47,'*',T60,'*',T80,'4',/,
     *T4,13('*'),T25,'VEL =',F9.1,T47,'*',T60,'*',T80,'5')
  820  FORMAT(T3,'*',T17,'*',T47,'*',T60,'*',T80,'6',/,
     *T2,'*',1X,'P0=',F8.1,T18,'*',T47,'*',T60,'*',T73,'PSYN=',T80,'7',/,
     *T2,'*',1X,'T0=',F8.1,'K',T18,'*',T33,14('*'),T60,'*',
     *T71,F6.0,'MM',T80,'8',/,
     *T2,'*',T18,'*',T29,4('*'),14('+'),T60,'*',T80,'9',/,
     *T2,'*',T18,'*',T25,'****',T33,'+',T46,'+',
     *T60,'*',T79,'10')
  830  FORMAT(T2,'*',T19,6('*'),T33,'+ HIZ=',F5.2,
     *'CM+',T51,'PCOLL=',T60,'*',T66,'***',T74,'*',T79,'11',/,
     *T2,'*',T16,'PT=',F6.1,T33,'+ WIZ=',F5.2,'CM+',T60,
     *6('*'),3X,7('*'),T79,'12',/,
     *T2,'*',T16,'RCRIT=',F5.3,1X,'—>',2X,'+ FRMACH=',F4.2,'+',
     *3X,F6.1,4X,'*',T66,'***',T74,'*',T79,'13',/,
     *T2,'*',T16,'TT=',F4.0,1X,'K',T33,'+ TEMP= ',F4.0,'K+',
     *T51,'TORR',T60,'*',4X,5('*'),T79,'14',/,
     *T2,'*',T33,'+ TORR=',F5.0,1X,'+',T60,'*',T79,'15')
  840  FORMAT(T2,'* WNOZ=',F6.1,'CM',2X,6('*'),T33,'+',T46,'+',T60,'*'
     *T79,'16',/,
     *T2,'* AFLOW=',F7.1,1X,'*',T25,'****',T33,'+IRRAD. ZONE +',
     *T60,'*',T65,'WCOMP=',T79,'17',/,
     *T2,'* ANOZ= ',F7.1,1X,'*',T29,4('*'),14('+'),T60,'*',T67,
     *F7.1,1X,'HP',T79,'18',/,
     *T2,'*',T18,'*',2X,'NOZZLE',T33,14('*'),T60,'*',T79,'19',/,
     *T2,'*',T18,'*',T47,'*',T60,'*',T79,'20')
  850  FORMAT(T3,'*',T17,'*',T47,'*',T60,'*',T79,'21',/,
     *T4,13('*'),T47,'*',T60,'*',T79,'22',/,
     *T9,'*',T47,'*  COLLECTOR *',T79,'23',/,
     *T8,'***',T48,'*',T59,'*',T79,'24',/,
     *T9,'*',T49,10('*'),T79,'25')
  860  FORMAT(T9,'*',T79,'26',/,
     *T8,'**',T79,'27',/,
     *T7,'*  * WTURB=',F7.1,1X,'HP',T79,'28',/,
     *T7,'*  *',T79,'29',/,
     *T8,'**',T79,'30')
  870  FORMAT(T8,'*',T79,'31',/,
     *T8,'* PCOAL=',F6.0,1X,'TORR',T79,'32'///)
      RETURN
      END
```

RELIABILITY, AVAILABILITY, MAINTAINABILITY ROUTINE

```
      SUBROUTINE RAM(OPTLIF,OPTREP,COLLIF,COLREP,AVAIL)
      COMMON/PRINT/ ITER,INTER,IPR
C     OPERATIONAL AVAILABILITY
      DATA ABERNY/0.987/
C     COMPRESSOR AVAILABILITY
      DATA AVCOMP/.999/
C     TURBINE AVAILABILITY
      DATA AVTURB/.995/
C     NOZZLE AVAILABILITY
      DATA AVNOZ/.993/
C     UTILITY AND SUPPORT AVAILABILITY
      DATA AVUTIL/.999/
C      LASER SYSTEM AVAILABILITY DUE TO OPTICAL ELEMENT FAILURE
      AVLAS=OPTLIF/(OPTLIF+OPTREP)
C     HS COLLECTOR
      AVCOLL=COLLIF/(COLLIF+COLREP)
C     AVAILABILITY FOR SERIES OF COMPRESSORS
      AVCOMT=AVCOMP**4
C     AVAILABILITY FOR SERIES OF THREE TURBINES
      AVTURT=AVTURB**3
C     TOTAL PLANT AVAILABILITY
      AVAIL=ABERNY*AVCOMT*AVTURT*AVNOZ*AVUTIL*AVLAS*AVCOLL
C     PRINT OUT
      IF(ITER.LE.IPR)
     1WRITE(6,112) OPTLIF,OPTREP,AVLAS,COLLIF,COLREP,AVCOLL,AVCOMP,
     1AVCOMT,AVTURB,AVTURT,AVNOZ,AVUTIL,ABERNY,AVAIL
  112 FORMAT(10X,'* * R.A.M. ANALYSIS & PLANT AVAILABILITY CALCULATION
     1 * *',//,10X,'LASER SYSTEM:OPTICS MTBF OF ',F6.1,' HR & MTTR OF '
     2,F6.2,' HR',/,10X,T24,'GIVES AVAILABILITY OF:',T52,F8.5,/,
     310X,'MS COLLECTOR:COLL MTBF OF ',F6.1,' HR & MTTR OF ',F6.2,' HR'
     4,/,T24,'GIVES AVAILABILITY OF:',T52,F8.5,/,10X,'COMPRESSORS:
     5SINGLE COMP; ',F8.5,' ; 4 COM',T52,F8.5,/,10X,
     6'TURBINES:SINGLE TURBINE; ',F8.5,' ; 3 TUR',T52,F8.5,/,
     710X,'NOZZLE:',T52,F8.5,/,10X,'UTILITIES & SUPPORT:',T52,F8.5,/,
     810X,'OPERATIONAL AVAILABILITY:',T52,F8.5,//,10X,'TOTAL PLANT
     9 AVAILABILITY:',T52,F8.5,//)
      RETURN
      END
```

ROUTINE TO CALCULATE PRESSURE RATIO IN NOZZLE

```
      SUBROUTINE PRATIO(HRAT,RCRIT,GAMMA,PRAT)
      REAL*4   K
      REAL*8 ROOT
      COMMON /PRINT/ ITER,INTER,IPR
      F(Y)=(K*(SQRT(1.-Y**EXPA))*Y**EXPB)-HRAT
      FF(Y)=(19189.*Y**0.7112*(-Y**0.2888+1.)**.5*
     *(2139.*Y**0.2888-1778.))/
     *(12500000.*Y*(Y**0.2888-1.))
      A=0.
      B=RCRIT
      EXPA=(GAMMA-1.)/GAMMA
      EXPB=1./GAMMA
      EXPC=0.5*(GAMMA+1.)/(GAMMA-1)
      K=1./((SQRT((GAMMA-1.)/2.))*((2./(GAMMA+1.))**EXPC))
      I=1
C     IF(ITER.LE.IPR)
C    1WRITE(6,30)
C  30 FORMAT(2X,'I',10X,'X',20X,'F(X)',20X,'FF(X)',/)
      X=.15
  200 ROOT=F(X)
      DIF=FF(X)
C     IF(ITER.LE.IPR)
C    1WRITE(6,10)I,X,ROOT,DIF
C  10 FORMAT(1X,I3,3(1X,F24.20),/)
      IF(DABS(ROOT).LE.1.E-8) GO TO 100
      B=X-(ROOT/DIF)
      X=B
      I=I+1
      IF(I.GT.40) GO TO 100
      GO TO 200
  100 CONTINUE
C     IF(ITER.LE.IPR)
C    1WRITE(6,20)X,ROOT
C  20 FORMAT(1X,'ROOT =',F24.20,3X,'F(X) =',F24.20)
      PRAT=X
      RETURN
      END
```

EXPANSION TURBINE DESIGN ROUTINE

```
      SUBROUTINE TURBIN(PCOAL,TCOAL,P0,T0,MOFLOW,MGAS,WTOT,QTOT,HPTOT,
     1TTO1)
      REAL*4 MOFLOW,MGAS
      COMMON/PRINT/ ITER,INTER,IPR
      CP=6.86
      TCOALR=TCOAL*1.8
      GAMMA=1.406
      R=1.98
      P0ATM=P0/760.
      PCOALA=PCOAL/760.
      PRATO=P0/PCOAL
C     USE THREE TURBINES WITH REHEATING OF GAS BETWEEN THEM
      TERM=(GAMMA/(GAMMA-1.))
      TERM1=1./TERM
      PR=PRATO**(1./3.)
      W1=MOFLOW*R*TCOALR*TERM*(1.-PR**TERM1)
      TTO1=TCOALR*(PR**TERM1)
      Q=MOFLOW*CP*(TCOALR-TTO1)
      WTOT=3.*W1
      QTOT=3.*Q
      HPTOT=(WTOT/(365.*24.*60.))/42.408
      IF(ITER.LE.IPR)
     1WRITE(6,101)PCOALA,P0ATM,TCOALR,TTO1,Q,QTOT,WTOT,HPTOT
  101 FORMAT(' TO OBTAIN POWER RECOVERY FOR POST PHOTOLYSIS RECOMPRES
     1SION',/,' THREE TURBINES ARE USED TO REDUCE PRESSURE FROM GASIF
     2IER AT ',F4.1,' ATM DOWN TO ',F4.2,' ATM',/,' AT NOZZLE PLENUM.
     3IN EACH TURBINE THE TEMPERATURE FALLS FROM ',F5.1,' R TO ',F5.1,
     4' R',/,' THUS REQUIRING ',E10.3,' BTU/YR OF REHEAT PER TURBINE
     5OR A TOTAL OF ',E10.3,' BTU/YR',/,' THE TOTAL TURBINE WORK AVAILAB
     6LE IS ',E10.3,' BTU/YR OR ',F9.1,' HP',//)
      RETURN
      END
```

COMPRESSOR DESIGN ROUTINE

```
      SUBROUTINE COMPRS(SCF,PCOLL,PSYN,MOFLOW,MGAS,HPNT,COSTT,QT,QAVAIL,
     1TEND,NCOMP)
      COMMON/PRINT/ ITER,INTER,IPR
      DIMENSION SVOL(4),HP(4),TOUT(4),SVOLN(4),HPN(4),Q(4),COST(4)
      REAL*4 MGAS,MOFLOW
      DATA SVOL/8.E4,2.81E4,9.4E3,3.5E3/
      DATA HP/9010.,9610.,9610.,9770./
      DATA TOUT/277.,295.,295.,299./
      CP=6.86
      GAMMA=1.406
      TIN=31.
      TIR=31.+460.
      TERM1=(GAMMA-1.)/(GAMMA*0.77)
      PCOLLA=PCOLL/760.
      PSYNA=PSYN/760.
      SCFB=9.1521E4
      SCFM=SCF/(365.*24.*60.)
      FACTOR=SCFM/SCFB
      DO 22 I=1,4
      SVOLN(I)=SVOL(I)*FACTOR
      HPN(I)=HP(I)*FACTOR
      Q(I)=MOFLOW*CP*(TOUT(I)-TIN)*0.89
   22 cost(I)=1.e6*(0.144159*alog((svoln(i)/1.e3))-3.04643e-5
     1*(svoln(i)/1.e3)**2+0.0167647*(svoln(i)/1.e3)+0.322085)
C    IF PCOLL<760 MM AN ADDITIONAL COMPRESSOR IS NEEDED
      IF(PCOLL.GE.760.) GO TO 30
      SVOLX=(760./PCOLL)*SVOL(1)*FACTOR
      PRX=PCOLL/760.
      HPX=HP(1)*(((1./PRX)**TERM1-1.)/(3.**TERM1-1.))*FACTOR
      TOUTX=TOUT(1)*(PRX**TERM1)
      QX=MOFLOW*CP*(TOUTX-TIN)*0.89
      COSTX=1.E6*((SVOLX/1.E4)**0.5)*0.707
      NCOMP=5
      GO TO 40
   30 HPX=0.
      QX=0.
      COSTX=0.
```

```
      TOUTX=TIN
      NCOMP=4
C   CASE WHERE PCOLL>760MM AND <2280MM
      IF(PCOLL.EQ.760.)GO TO 40
      SVOLN(1)=(760./PCOLL)*SVOL(1)*FACTOR
      PRX=760/PCOLL
      HPN(1)=HP(1)*(((1./PRX)**TERM1-1.)/(3.**TERM1-1.))*FACTOR
      TOUT(1)=TOUT(1)*(PRX**TERM1)
      Q(1)=MOFLOW*CP*(TOUT(1)-TIN)*0.89
      COST(1)=1.E6*((SVOLN(1)/1.E4)**0.5)*0.707
   40 HPNT=HPX+HPN(1)+HPN(2)+HPN(3)+HPN(4)
      QT=QX+Q(1)+Q(2)+Q(3)+Q(4)
      COSTT=COSTX+COST(1)+COST(2)+COST(3)+COST(4)
      QAVAIL=Q(4)
      TEND=TOUT(4)
      IF(ITER.LE.IPR)
     1WRITE(6,102) SCFM,PCOLLA,PSYNA,TIR
  102 FORMAT(' FOUR OR MORE COMPRESSORS ARE REQUIRED TO RECOMPRESS ',
     1F9.1,' SCFM',/,' OF SYNGAS FROM THE COLLECTION ZONE PRESSURE
     2 OF ',F6.2,' ATM BACK INTO',/,' THE METHANOL SYNTHESIZER AT ',
     3F6.2,' ATM.   INPUT GAS TEMPERATURE IS ',F6.1,' R',///)
      IF(ITER.LE.IPR)
     1WRITE(6,103)
  103 FORMAT(' COMPR. #   SUCTION VOL.   OUTPUT T   REQD COOLING   POWER
     1          COST',/
     2       ,'              (CFM)            (F)        (BTU/YR)       (HP)
     3          ($MM)',/)
      I=1
      IF(ITER.LE.IPR)
     1WRITE(6,104) SVOLX,TOUTX,QX,HPX,COSTX
  104 FORMAT(' ',T13,F10.1,5X,F5.1,6X,E9.2,4X,F8.1,3X,F9.0,/)
      IF(ITER.LE.IPR)
     1WRITE(6,105) I,SVOLN(1),TOUT(1),Q(1),HPN(1),COST(1)
      I=2
      IF(ITER.LE.IPR)
     1WRITE(6,105) I,SVOLN(2),TOUT(2),Q(2),HPN(2),COST(2)
      I=3
      IF(ITER.LE.IPR)
     1WRITE(6,105) I,SVOLN(3),TOUT(3),Q(3),HPN(3),COST(3)
      I=4
      IF(ITER.LE.IPR)
     1WRITE(6,105) I,SVOLN(4),TOUT(4),Q(4),HPN(4),COST(4)
  105 FORMAT(' ',I1,T13,F10.1,5X,F5.1,6X,E9.2,4X,F8.1,3X,F9.0,/)
      IF(ITER.LE.IPR)
     1WRITE(6,107)
  107 FORMAT(' ',T14,'-------------------------------------------------
     1---------',/)
      IF(ITER.LE.IPR)
     1WRITE(6,108) QT,HPNT,COSTT
  108 FORMAT(' ',T39,E9.2,4X,F8.1,3X,F9.0,///)
      RETURN
      END
```

ENERGY MANAGEMENT ROUTINE

```
      SUBROUTINE ENERGY(WTURB,WCOMP,TOUT,QAVAIL,QT,QTOT,TTO1,TSYN,MGAS,
     1MOFLOW,SREQCP,SREQME,KWHR,ATURB,ACOMP,AMEX,TONS,GPM,KWPUMP,KWREFR,
     2SREQ,KWEQUI,KW)
      REAL*4 MGAS,MOFLOW,KW,KWHR,KWEQUI,KWPUMP,KWREFR
      COMMON /PRINT/ITER,INTER,IPR
C     CALCULATION OF THERMAL ENERGY REQUIREMENTS
C     HEAT CAPACITY OF SYNGAS
      CP=6.86
C     STEAM RATE FOR TURBINE DRIVEN COMPRESSORS. INLET STEAM @ 600PSIA,
C     1000 F. UNITS ARE LB STEAM/HP-HR
      SRATE=6.51
C     HEAT VALUE OF 600 PSIA ,1000 F STEAM AVAILABLE TO HEAT SYNGAS
C     FROM 295 F TO 448 F IN BTU/LB STEAM
      HSTM=1086.
C     CALCULATION OF COMPRESSOR STEAM REQUIREMENTS(LB/YR)
      KWEQUI=WCOMP*0.745*0.85
      HPHR=WCOMP*365.*24.
      SREQCP=HPHR*SRATE
C     CALCULATION OF STEAM TO HEAT SYNGAS INTO METHANOL UNIT(LB/YR)
      QREQME=MOFLOW*CP*(TSYN-TOUT)
      SREQME=QREQME/HSTM
C     HEAT EXCHANGER REQUIREMENTS
C     TURBINE EXHAUST REHEATERS
C     HEAT LOAD PER EXCHANGER
      QTURB=QTOT/3.
C     HEAT EXCH. COEFF.(LIQ COOLANT) IN BTU/HR*FT2*DEGF
      U=300.
C     AVE H-X DELTA T
      DELT=70.*(TTO1/442.)
C     HOURLY LOAD
      QX=QTURB/8760.
C     REQUIRED H-X AREA(FT2)
      ATURB=QX/(U*DELT)
C     COMPRESSOR COOLERS
C     HOURLY HEAT LOAD FOR ALL COMP. COOLERS(UNITS 1-3)
      QQ=QT-QAVAIL
      QC=QQ/8760.
C     USE SAME U AS FOR TURBINE REHEATER
C     AVERAGE H-X DELTA T
      DELTAT=80.*(TOUT/295.)
C     REQUIRED AREA(FT2)
      ACOMP=QC/(U*DELTAT)
C     HEATUP OF SYNGAS PRIOR TO METHANOOL REACTOR
C     HEAT EXCHANGE COEF.(COND.STEAM)
      UU=1000.
C     HOURLY LOAD
      QME=QREQME/8760.
C     AVERAGE H-X DELTA T
      DELTT=120.*(TOUT/295.)
C     H-X AREA CALCULATION
```

```
      AMEX=QME/(UU*DELTT)
C     SPECIFIC HEAT OF COOLANT
      CPLIQ=0.4
C     COOLING LIQUID FLOWRATE(COMPRESSORS)
      FLCCUL=QC/(CPLIQ*180.)
C     HEATING LIQ. FLOWRATE(TURBINES)
      FLTCUL=QTOT/(CPLIQ*80.*8760.)
      FMK=FLCCUL-FLTCUL
C     TONS OF REFRIGERATION REQUIRED TO COOL COOLANT TO COMPRESSORS
      TONS=((QQ/(8760.*60.))/200.)*(100./180.)
C
C     ELECTRICAL ENERGY
C     ELECTRICITY PRODUCED FROM TURBINES
      KW=(WTURB*.745)*0.85
      KWHR=KW*8760. ,
C     ELECTRICITY TO DRIVE CENTRIFUGAL COOLANT PUMPS FOR HEAT EXCHRS
      GPM=(FLCCUL+FLTCUL)/(60.*8.33)
      HPCENT=40.*GPM/(3960.*0.8)
      KWPUMP=HPCENT*0.745/0.95
C     ELECTRIC POWER FOR REFRIGERATION
      HPTON=0.925
      HPREFR=0.925*TONS
      KWREFR=0.745*HPREFR/0.95
C     TOTAL STEAM REQTS
      SREQ=SREQCP+SREQME
      IF(ITER.LE.IPR)
     1WRITE(6,200)
  200 FORMAT('0   HEAT EXCHANGE AND ENERGY REQUIREMENTS',/)
      IF(ITER.LE.IPR)
     1WRITE(6,201) WCOMP,KWEQUI,QT,QAVAIL,QQ,FLCCUL,ACOMP,QC,
     1SREQCP,TONS
  201 FORMAT('     ***TOTAL COMPRESSOR POWER:',T68,F10.1,' HP'
     1,/,'          (',F9.1,' KW ELECT. EQUIV.)',
     2/,' HEAT PRODUCED BY STEAM TURBINE DRIVEN COMP.:(BTU/YR)',T68,E10.
     33,/,' PORTION USED TO PARTIALLY REHEAT SYNGAS(LAST COMP)',T68,E10.
     43,/,' PORTION WHICH MUST BE REMOVED BY HEAT EXCHANGERS',T68,E10.3,
     5/,' LB OF COOLANT PER HOUR REQUIRED',T68,E10.3,
     6/,' TOTAL HEAT EXCHR TUBE AREA REQD(FT2)',T68,F10.0,
     6/,' HOURLY HEAT EXCHANGER LOAD(BTU/HR)',T68,E10.3,
     7/,' STEAM REQT FOR COMPRESSORS(LB/YR @600PSIA,1000F)',T68,E10.3,
     8/,' REFRIGERATION LOAD TO RECOOL COMPRESSOR COOLANT(TONS)',T68,
     9F10.0,//)
      IF(ITER.LE.IPR)
     1WRITE(6,202) WTURB,KW,QTURB,FLTCUL,ATURB,QX
  202 FORMAT('     ***TOTAL POWER PRODUCED BY EXPANSION TURBINES:',T50,
     1F10.0,' HP   OR',T68,F10.0,'KW',
     2/,' REHEAT REQTS FOR EACH OF THREE TURBINES',T68,E10.3,
     3/,' LB OF HEAT TRANSFER FLUID PER HOUR(ALL TURBINES)',T68,E10.3,
     4/,' HEAT EXCHR TUBE AREA PER TURBINE REHEATER(FT2)',T68,F10.0,
     5/,' HOURLY HEAT EXCHANGER LOAD PER TURBINE(BTU/HR)',T68,E10.3,
     6//)
```

```
      IF(ITER.LE.IPR)
     1WRITE(6,203) TOUT,TSYN,SREQME,AMEX,QME
  203 FORMAT('      ***POST COMPRESSION REHEAT OF SYNTHESIS GAS FROM',
     1F5.0,' TO ',F5.0,' F',/,' STEAM REQUIREMENT(LB/YR : 600PSIA,1000F)
     2',T68,E10.3,/,' HEAT EXCHANGER AREA REQUIRED(FT2)',T68,F10.0,/,
     3 ' HOURLY HEAT EXCHANGER LOAD(BTU/HR)',T68,E10.3,///)
      IF(ITER.LE.IPR)
     1WRITE(6,204) GPM,HPCENT,KWPUMP,HPREFR,KWREFR
  204 FORMAT('      ***ELECTRIC POWER USE-COOLANT PUMPS & REFRIGERATION:'
     1,/,' TOTAL CENTRIFUGAL PUMP CAPACITY OF ',E10.3,'GPM REQUIRES',/,
     2' HYDRAULIC HP OF ',F9.3,' OR ',F9.3,' KW ELECTRIC.',/,
     3' CHILLER/REFRIG FOR COMPRESSOR COOLANT REQUIRES ',F9.3,' HP
     4OR ',F9.3,' KW',//)
      RETURN
      END
```

LASER SYSTEM DESIGN ROUTINE

```
      SUBROUTINE LASDES(REPMAX,REP,PHIUV,XCBEAM,POWMAX,POWHD,
     1POWHDB,NHEAD,NSETS,NHDSET)
      REAL*4 MOSULF,MOSULB,MOFLOW,MOFLWB
      COMMON/PRINT/ ITER,INTER,IPR
C     LASER SYSTEM DESIGN AND ARCHITECTURE
C     NO. OF LASER SETS REQD TO OBTAIN REP RATE
      NSETS=REP/REPMAX+0.99
C     LASER OUTPUT POWER PER SET
      SETPOW=REPMAX*PHIUV*XCBEAM
C     NUMBER OF LASER HEADS PER LASER SET( > 1 IF LASER SET OUTPUT
C     IS > POWMAX
      NHDSET=SETPOW/POWMAX+0.99
C     OUTPUT POWER PER LASER HEAD
      POWHD=SETPOW/NHDSET
C     TOTAL # OF LASER HEADS
      NHEAD=NHDSET*NSETS
C     PRINT OUT
      IF(ITER.LE.IPR)
     1WRITE(6,300) REPMAX,REP,NSETS,SETPOW
  300 FORMAT('0IF A SINGLE LASER HEAD IS LIMITED TO A',
     1/,' PRF OF ',-3PF6.3,' KHZ, THE SYSTEM PRF OF ',-3PF6.3,
     2/,' KHZ REQUIRES ',I2,' LASER SETS AT AN OUTPUT POWER OF',
     3/,' ',-3PF6.3,'KW EACH.',/)
      IF(ITER.LE.IPR)
     1WRITE(6,301) POWMAX,NHDSET,POWHD,NHEAD
  301 FORMAT(' A SINGLE LASER HEAD IS LIMITED TO AN
     1 OUTPUT POWER OF ',-3PF6.3,' KW',/,' THE NUMBER
     2 OF LASER HEADS PER LASER SET IS ',I2,' AT ',-3PF6.3,
     3' KW PER HEAD.',/,' THE TOTAL NUMBER OF HEADS IN THE LASER
     4 SYSTEM IS ',I2,/)
      RETURN
      END
```

PLANT EQUIPMENT LAYOUT ROUTINE

```
      SUBROUTINE LAYOUT(WNOZ,WTURB,WTURBB,WCOMP,WCOMPB,NHEAD,POWHD,
     1POWHDB,MOSULF,MOSULB,MOFLOW,MOFLWB,ATOT)
      REAL*4 MOSULF,MOSULB,MOFLOW,MOFLWB
      COMMON/PRINT/ ITER,INTER,IPR
C
C EQUIPMENT FLOOR AREAS NEEDED TO SIZE ADDTL.BUILDING SPACE
C    NOZZLE AND PHOTOLYSIS REACTOR REGION
      ANOZF=50.*(WNOZ/30.48+5.)
C   TURBINE AND GENERATOR AREA
      ATURBI=40.*95.*(WTURB/WTURBB)**0.6
C   COMPRESSOR REGION
      ACOMPR=35.*120.*(WCOMP/WCOMPB)**0.6
C   LASER AREA(APPROX 40FT2/LASER HEAD)
      ALASR=40.*NHEAD*(POWHD/POWHDB)**0.5
C   BEAM HANDLING AREA
      ABEAM=20.*NHEAD
C   COLLECTOR REFURB AREA
      ACOLL=2500.*(MOSULF/MOSULB)
C   TANK STORAGE AREA
      ATANK=1200.*(MOFLOW/MOFLWB)**0.666
C   PROCESS SUPPORT AREA
      APSA=1250.*(MOFLOW/MOFLWB)
C   TOTAL ADD-ON BLDG AREA IN FT2
      ATOT=ANOZF+ATURBI+ACOMPR+ALASR+ABEAM+ACOLL+ATANK+APSA
C   PRINT OUT
      IF(ITER.LE.IPR)
     1WRITE(6,302)ANOZF,ATURBI,ACOMPR,ALASR,ABEAM,ACOLL,ATANK,APSA,
     1ATOT
  302 FORMAT(T25,' * * * PLANT AREA ESTIMATES * * *',/
     *10X,'PLENUM,IRRADIATION ZONE,COLLECTOR',T52,F12.0,/,
     *10X,'EXPANSION TURBINES & REHEATERS &GENERATORS',T52,F12.0,/,
     *10X,'COMPRESSORS,COOLERS,&MOTORS',T52,F12.0,/,
     *10X,'LASER SYSTEM,INCL. POWER CONDITIONING',T52,F12.0,/,
     *10X,'BEAM HANDLING EQPT',T52,F12.0,/,
     *10X,'COLLECTOR REFURBISHMENT',T52,F12.0,/,
     *10X,'SYNGAS STORAGE TANKS',T52,F12.0,/,
     *10X,'PROCESS SUPPORT',T52,F12.0,/,
     *10X,T52,12('-'),/,
     *10X,'TOTAL ADD-ON BLDG AREA  (FT2)',T52,F12.0,////)
      RETURN
      END
```

ELECTRICAL POWER USAGE ROUTINE

```
      SUBROUTINE ELECTR(KW,KWPUMP,KWREFR,WALLPG,AVAIL,ATOT,POWRI,
     1POWRO,KWEQUI,KWTOT,KWUSE,KWCAP)
      REAL*4 KW,KWPUMP,KWREFR,KWHV,KWLI,KWIC,KWRCW,KWTOT,KWEQUI,
     1KWUSE,KWLAS,KWNET,KWLIO,KWHVO,KWRCWO,KWCAP
      COMMON/PRINT/ITER,INTER,IPR
      POWRF=0.9
      CF=AVAIL
C   OTHER ELECTRIC POWER
C    LASER
      KWLAS=WALLPG/1.E3
C   INS& CONTROL
      KWIC=100.
C    LIGHTING
      KWLI=.0017*ATOT
      KWLIO=KWLI/CF
C    HEATING AND VENTILATION
      KWHV=.00823*ATOT
      KWHVO=KWHV/CF
C    RECIRC COOLING WATER PUMPS
      KWRCW=.021*(KWEQUI+KW)
      KWRCWO=KWRCW/CF
C   TOTALS
      KWUSE=KWPUMP+KWREFR+KWLAS+KWIC+KWLIO+KWHVO+KWRCWO
      KWCAP=(KWPUMP+KWREFR+KWLAS+KWIC+KWLI+KWHV+KWRCW)/POWRF
C   NET POWER USE OR PRODUCTION
      KWNET=KW-KWUSE
      POWRO=KWNET/1.E3
      POWRI=KWCAP/1.E3
C   PRINT OUT
      IF(ITER.LE.IPR)
     1WRITE(6,222)KWLAS,KWPUMP,KWREFR,KWIC,KWLIO,KWHVO,KWRCWO,KWUSE,
     1KW,KWNET,KWCAP
  222 FORMAT(10X,'* * ELECTRIC POWER CONSUMPTION & PRODUCTION IN KW * *'
     1,/,10X,'LASERS',T44,F10.2,/,
     210X,'CENTRIFUGAL COOLANT PUMPS',T44,F10.2,/,
     *10X,'REFRIGERATION',T44,F10.2,/,
     *10X,'INSTR.&CONTROLS',T44,F10.2,/,
     *10X,'LIGHTING',T44,F10.2,/,
     *10X,'HEATING & VENTILATION',T44,F10.2,/,
     *10X,'RECIRC. WATER SYSTEM',T44,F10.2,/,
     *10X,T44,'----------',/,
     *10X,'TOTAL OPERATING POWER CONSUMED',T44,F10.2,/
     *10X,'ELECT PROD FROM TURBINES',T44,F10.2,/,
     *10X,'NET POWER USE OR PRODUCTION',T44,F10.2,//,
     *10X,'TOTAL INSTALLED CAPACITY',T44,F10.2,/,10X,'(POWER
     * CONSUMING HARDWARE ONLY)',//)
      RETURN
      END
```

CAPITAL COST SCALING ROUTINE

```
      SUBROUTINE CAPCOS(WNOZ,WTURB,WTURBB
     1,NCOMP,POWHDB,MOSULB,MOSULF,MOFLOW,MOFLWB,CCPWAT,
     2COSTT,WATTAV,ACOMP,HPNT,ATURB,TONS,AMEX,CTOT,SCFM,P0,GPM,NHEAD,
     3NHEADB,WALLPG,ATOT,POWRI,SREQ,KWCAP,KWCAPB,CLRCC,CGH,COUNIT,
     4CLUNIT,FCOG,FPDF)
      REAL*4 MOSULF,MOSULB,MOFLOW,MOFLWB,KWCAP,KWCAPB
      COMMON/PRINT/ ITER,INTER,IPR
C   COST ESCALATION FACTORS
C    1978 TO MID 1982
      E1=1.46
C COST SCALING EQUATIONS
C   NOZZLE,PLENUM,PHOTOLYSIS CHAMBER,& COLL COST
      CNOZ=200.*WNOZ
C   SPARE COLLECTOR UNITS
      CLSPR=CLUNIT*10.
C   LASER SYST CAPITAL COST
      CLASR=CCPWAT*WATTAV
C   BEAM TRANSPORT SYSTEM COST
      CBEAM=0.2*CLASR
C   OPTICAL MULTIPLEXER COST
      CMPXR=1.E5*(NHEAD/NHEADB)
C   SPARE OPTICAL UNITS
      COSPR=COUNIT*5.
C   TURBINE COST
      CTUR=E1*48.*(WTURB/3.)**0.93
      CTURB=3.*CTUR
C   GENERATOR COSTS
      CGEN=E1*1.5*3.*20.*(WTURB/3.)**0.93
C   TURBINE REHEATER COST
      CHEXT=E1*3.*70.8*ATURB**0.83
C   COMPRESSOR COST
      CCOMP=COSTT
C   COMPRESSOR TURBINES(STEAM DRIVEN)
      CMOTC=E1*NCOMP*48.*(HPNT/NCOMP)**0.93
C   COMPRESSOR COOLERS
      CCCUL=E1*(NCOMP-1)*70.8*(ACOMP/(NCOMP-1))**0.83
C   REFRIGERATOR FOR COMPRESSOR COOLANT
      CREFR=E1*1717.*(TONS**0.665)
```

```
C   HEAT EXCHANGER FOR POST COMPRESSION REHEAT
      CMEX=E1*70.8*AMEX**0.83
C   PIPING COST
      CPIPE=E1*4.*SCFM**0.7
C   SYNGAS STORAGE TANK COST
      VOL=SCFM*(760./P0)*2.
      DIA=1.24*(VOL**(1./3.))
      PP=(P0/760.)*14.7
      SCALE=(DIA**2)*SQRT(PP)
      CTANK=E1*15.27*SCALE**0.95
C   PUMPS FOR HEAT EXCHANGE FLUID
      HEAD=40.
      QH=GPM*HEAD
      CPUMPS=E1*0.32*QH
C   INSTRUMENTATION AND CONTROL
      CIC=1.E5*(NHEAD/NHEADB)
C   PRE-OPERATIONAL CHECKOUT
      CPCHK=76.E3+50.*WNOZ
C   COOLING WATER SYSTEM FOR LASERS
      COW=2.E5*(WALLPG/3.64E6)**0.7
C   OUTSIDE UTILITIES(INCL. SWITCHGEAR)
      COUTS=.001*POWRI+.001*SREQ
C   SPECIAL SHOPS
      CSS=50.E3*(MOSULF/MOSULB)
C   ELECTRICAL DIST SYSTEM
      CEDS=40.E3*(KWCAP/KWCAPB)
C   BUILDING COST
      CBLDG=120.*ATOT
C   TOTAL DIRECT COST
      CCTOT=CNOZ+CLASR+CBEAM+CTURB+CGEN+CHEXT+CCOMP+CMOTC+CCOUL
     1+CREFR+CMEX+CBLDG+CTANK+CPUMPS+COW+CIC+CPCHK+COUTS+CPIPE+
     2CSS+CEDS+CMPXR+COSPR+CLSPR
C   INDIRECT COSTS
C    ENGINEERING
      ENGRG=0.25
      CENG=ENGRG*CCTOT
      C1TOT=CCTOT+CENG
C   CONTINGENCY ANALYSIS
C    LASER EQUIPMENT
      FCONL=0.5
      CONL=FCONL*(CLASR+CBEAM+COW+CIC+CMPXR+COSPR)
C    GAS HANDLING EQUIPMENT
      FCONGH=0.3
      CONGH=FCONGH*(CNOZ+CTURB+CGEN+CHEXT+CCOMP+CCOUL+CMEX+
     1CTANK+CPIPE+CSS+CLSPR)
C    BALANCE OF PLANT
      FCONBP=0.3
      CONBP=FCONBP*(CMOTC+CREFR+CPUMPS+CPCHK+COUTS+CEDS+CBLDG)
C    COMPOSITE CONTINGENCY
      CONTOT=CONL+CONGH+CONBP
      FCONAV=CONTOT/CCTOT
```

```
      CONTT=FCONAV*C1TOT
C     SUMMATION
      C2TOT=CONTT+C1TOT
C     INTEREST DURING CONSTRUCTION
      RIDC=0.1
      FADD=RIDC*(FPDF-1.)*C2TOT
      CIDC=RIDC*C2TOT
C     SUMMATION AND CALC OF TOTAL PLANT CAPITAL
      CTOTS=(C2TOT+CIDC+FADD)
      CCOG=(FCOG-1.)*CTOTS
      CTOT=CCOG+CTOTS
C     LASER RELATED CAPITAL COSTS
      FACTO=FCOG*(1.+ENGRG)*(1.+FCONC)*(1.+RIDC)
      CLRCC=FACTO*(CLASR+CBEAM+CIC+CCW+CMPXR+COSPR+0.5*(CBLDG+CEDS))
C     GAS HANDLING RELATED COSTS
      CGH=FACTO*(CNOZ+CTURB+CGEN+CHEXT+CCOMP+CMOTC+CCOUL+CREFR+
     1CPIPE+CTANK+CPUMPS+CLSPR+0.5*(CBLDG+CEDS))
C     PRINT OUT
      IF(ITER.LE.IPR)
     1WRITE(6,405)
  405 FORMAT(T10,'* * * PLANT CAPITAL COST ESTIMATE * * THOUSANDS OF $',
     *//)
      IF(ITER.LE.IPR)
     1WRITE(6,401) CNOZ,CLSPR,CLASR,CBEAM,CMPXR,COSPR
  401 FORMAT(10X,'NOZZLE,PLENUM,DISCH.SECT.&INIT.COLL.',T52,-3PF12.3,/,
     *10X,'SPARE COLLECTOR UNITS',T52,-3PF12.3,/,
     *10X,'LASER SYSTEM',T52,-3PF12.3,/,
     *10X,'BEAM TRANSPORT SYSTEM',T52,-3PF12.3,/,
     *10X,'OPTICAL MULTIPLEXER',T52,-3PF12.3,/,
     *10X,'SPARE OPTICAL UNITS',T52,-3PF12.3,/)
      IF(ITER.LE.IPR)
     1WRITE(6,402)CTURB,CHEXT,CGEN
  402 FORMAT(10X,'EXPANSION TURBINES',T52,-3PF12.3,/,
     *10X,'TURBINE REHEATERS',T52,-3PF12.3,/,
     *10X,'TURBINE GENERATORS',T52,-3PF12.3,/)
      IF(ITER.LE.IPR)
     1WRITE(6,403)CCOMP,CMOTC,CCOUL,CREFR,CMEX,CTANK,CPUMPS,CCW,CIC,
     1CPCHK,COUTS,CSS,CEDS,CPIPE
  403 FORMAT(10X,'COMPRESSORS',T52,-3PF12.3,/
     *10X,'COMPRESSOR STEAM TURBINES',T52,-3PF12.3,/,
     *10X,'COMPRESSOR COOLERS',T52,-3PF12.3,/,
     *10X,'REFRIGERATION FOR COMPRESSOR COOLANT',T52,-3PF12.3,/,
     *10X,'HEAT EXCHR. FOR POST COMP.REHEAT',T52,-3PF12.3,/,
     *10X,'STORAGE TANK FOR PLENUM SYNGAS',T52,-3PF12.3,/,
     *10X,'HEAT EXCHANGER COOLANT PUMPS',T52,-3PF12.3,/,
     *10X,'COOLING WATER SYSTEM FOR LASERS',T52,-3PF12.3,/,
     *10X,'INSTRUMENTATION AND CONTROL',T52,-3PF12.3,/,
     *10X,'PRE-OPERATIONAL CHECKOUT',T52,-3PF12.3,/,
     *10X,'OUTSIDE UTILITIES(INCL. SWITCHGEAR)',T52,-3PF12.3,/,
     *10X,'SPECIAL SHOPS(INCL.COLL.REFAB)',T52,-3PF12.3,/,
```

```
     *10X,'ELECTRICAL DISTRIBUTION SYSTEM',T52,-3PF12.3,/,
     *10X,'SYSTEM PIPING',T52,-3PF12.3,/)
      IF(ITER.LE.IPR)
     1WRITE(6,404)CBLDG,CCTOT
  404 FORMAT(10X,'BUILDING',T52,-3PF12.3,/,
     *10X,T52,'------------',/,
     *10X,'SUBTOTAL',T52,-3PF12.3,//)
      IF(ITER.LE.IPR)
     1WRITE(6,406)ENGRG,CENG,C1TOT,FCONAV,CONTT,C2TOT,RIDC,CIDC,
     1FPDF,FADD,CTOTS,FCCG,CCCG,CTOT
  406 FORMAT(10X,'ENGINEERING AT ',2PF6.3,' % OF DIRECT COSTS',T52,
     *-3PF12.3,/,T52,'------------',/,10X,'SUBTOTAL',T52,-3PF12.3,/,
     *10X,'CONTINGENCY AT ',2PF6.3,' % OF ABOVE',T52,-3PF12.3,/,
     *T52,'------------',/,10X,'SUBTOTAL',T52,-3PF12.3,/,
     *10X,'INTEREST DURING CONSTRUCTION AT ',2PF6.3,' %',T52,-3PF12.3,
     */,10X,'ADDTL IDC DUE TO FPDF OF  ',0PF5.3,T52,-3PF12.3,
     */,T52,'------------',/,10X,'TOTAL CAPITAL COST',T52,-3PF12.3,//
     *,10X,'ADDTL CAP COST DUE TO FCCG OF  ',0PF5.3,T52,-3PF12.3,/
     *,T52,'----------',/,10X,'TOTAL ADJUSTED CAPITAL COST',T52,
     *-3PF12.3,//)
      RETURN
      END
```

STAFFING ROUTINE

```
      SUBROUTINE LABOR(MOFLOW,MOFLWB,OPTLIF,COLLIF,NSTAFF,
     1AVAIL,SALTOT,OPRATE,CLRATE,POWHD,POWHDB)
      REAL*4 MOFLOW,MOFLWB
      COMMON/PRINT/ ITER,INTER,IPR
C     ANNUAL SALARIES FOR MONTHLY,WEEKLY TECH,WEEKLY CLERICAL,&HOURLY
C     LABOR
      DATA PAYS/34000./,PAYWT/22000./,PAYWC/14000./,PAYH/20000./
C     OPTICAL UNITS PER YEAR REPAIRED
      OPRATE=(8760./OPTLIF)*AVAIL
C     COLLECTORS PER YEAR CLEANED AND REFABRICATED
      CLRATE=(8760./COLLIF)*AVAIL
C     NUMBER OF SHIFTS
      NSHIFT=5
C     ASSUME ONE MAN PER SHIFT CAN REPAIR AND REPLACE 50 OPTICAL UNITS
C     PER YEAR(BASE CASE: COULD BE MORE OR LESS DEPENDING ON POWHD)
      NOPFIX=50*(POWHDB/POWHD)
      NOPMAN=OPRATE/(NSHIFT*NOPFIX)+.99
      NOPMNT=NSHIFT*NOPMAN
C     ASSUME ONE MAN PER SHIFT CAN REFABRICATE 100 COLLECTORS PER YR
      NCLFIX=100.
      NCLMAN=CLRATE/(NSHIFT*NCLFIX)+.99
      NCLMNT=NSHIFT*NCLMAN
C     SUPERVISORS: 1 PER SHIFT
      NSUPER =NSHIFT
C     SUPPORT PERSONNEL(DAYSHIFT ONLY)
      NSUPP2=(MOFLOW/MOFLWB)+.99
      NSUPP3=(MOFLOW/MOFLWB)+.99
C TOTAL STAFF
      NSTAFF=NOPMNT+NCLMNT+NSUPER+NSUPP2+NSUPP3
C     STAFF BY SALARY CATEGORY
C      MONTHLY SALARIED(SUPERVISORY)
       NMONTH=NSUPER
       SALM=NMONTH*PAYS
C      WEEKLY TECHNICAL
       NWTEK=NSUPP2
       SALWT=NWTEK*PAYWT
C      WEEKLY CLERICAL
       NWKCLR=NSUPP3
       SALWC=NWKCLR*PAYWC
C      HOURLY LABOR
       NHRLY=NOPMNT+NCLMNT
       SALH=PAYH*NHRLY
C      TOTAL BASE LABOR
       SALTOT=SALM+SALWT+SALWK+SALH
```

```
C     PRINT OUT
       IF(ITER.LE.IPR)
     1WRITE(6,101)NMONTH,SALM,NHRLY,SALH,NWTEK,SALWT,
     1NWKCLR,SALWC,NSTAFF,SALTOT
  101 FORMAT(10X,'* * * STAFFING TABLE &COSTS FOR 5 SHIFT OPERATION * *
     1 *',//,10X,'CATEGORY',T30,'# OF EMPLOYEES ',T52,'LABOR COST',/,
     210X,T28,'(M)   (WT)   (WC)   (H)',T50,'($ THOUSANDS)'//,10X,
     3'SUPERVISORY';T28,I2,T52,-3PF9.3,/,10X,'E-O SYSTEM REPAIR &',/,
     410X,'COLLECTOR REFURB',T44,I3,T52,-3PF9.3,/,10X,
     5'TECHNICAL SUPPORT',T33,I2,T52,-3PF9.3,/,10X,'CLERICAL SUPPORT',
     6T39,I2,T52,-3PF9.3,/,T52,'----------',/,10X,'TOTAL COST FOR A
     8STAFF OF ',I3,T52,-3PF9.3,
     7///)
      RETURN
      END
```

OPERATING COST SCALING AND FIGURES OF MERIT ROUTINE

```
      SUBROUTINE OPRCOS(FEEDKG,MOPHOT,WALLPG,WATTAV,SCUT,KGSULF,SCF,
     1SREQCP,SREQME,KWHR,CCPWAT,CTOT,KWUSE,POWRO,AVAIL,OPTLIF,
     2COLLIF,NSTAFF,SALTOT,OCPWAT,COUNIT,CLUNIT,KWCAPB,KWCAP,ATOT,
     3ATOTB,MOFLOW,MOFLWB,OPRATE,CLRATE,CLRCC,CGH,MFSULF,EVPHOT,MOSULF,
     4MWN,ANCOST,CPHOT,COGH,CUNIT,PERCT,TON,FPD,FCOG,FOCG,FPDF)
      REAL*4 MOPHOT,METHC,KGSULF,KWHR,KWL,KWN,MWT,MWL,MWN,MWU,KWUSE,
     1MOFLOW,MOFLWB,KWCAP,KWCAPB,MFSULF,KWHUSE,MOSULF
      COMMON /PRINT/ ITER,INTER,IPR
      DATA FPCT/0.25/,CLPCT/0.20/,CAPREC/0.1102/
C     COST OF MED. BTU SYNGAS PER MILLION BTU
      CSYNGS=7.2
C     ANNUAL OPERATING COST OF METHANOL PLANT(EXCL CLAUS PLANT AND ZNO
      COPME=14.2494E6                                  OR LASER S REMOVAL)
C     COST OF 600LB STEAM PER 1000 LBS
      CSTM=2.90
C     STEAM TO DRIVE COMPRESSORS:
      CSTMCP=(SREQCP/1.E3)*CSTM
C     STEAM TO HEAT SYNGAS PRIOR TO MEOH REACTOR
      CSTMME=(SREQME/1.E3)*CSTM
C     TOTAL STEAM COST
      CSTMT=CSTMCP+CSTMME
C     PRINT OUT STEAM CALCULATIONS
      IF(ITER.LE.IPR)
     1WRITE(6,18)CSTM,SREQCP,CSTMCP,SREQME,CSTMME,CSTMT
   18 FORMAT(10X,'STEAM REQTS & ANNUAL COSTS AT',F6.2,' PER THOUSAND LB:
     1',/,10X,'STEAM TURBINE DRIVEN COMPRESSORS: ',5X,-0PE10.3,' LB/YR',
     2T66,-3PF9.2,/,10X,'REHEAT OF SYNGAS PRIOR TO MEOH REACTOR:',-0PE10
     3.3,' LB/YR',T66,-3PF9.2,//,10X,'TOTAL STEAM COST',T66,-3PF9.2,//)
      FRACTM=1.
C     FRACTION OF SYNGAS CONVERTED TO METHANOL
      FEEDRQ=FEEDKG*AVAIL
      CH3OH=FRACTM*FEEDKG*AVAIL
C     DAILY MEOH PRODUCTION
      DAILY=(CH3OH/1.E3)*1.1025/365.
C     HOURLY MEOH PRODUCTION(DESIGN)
      HRLY=(DAILY/24.)/AVAIL
C     ACTUUAL HOURLY MEOH PRODUCTION
      HRLYO=HRLY*AVAIL
C     POWER CONVERSIONS AND COST
      CPOWER=.030
```

```
      MWT=KWHR/(8760.*1.E3)
      MWL=WALLPG/1.E6
      MWU=KWUSE/1.E3
      KWHUSE=KWUSE*8760.
      MWN=MWU-MWT
      KWL=8760.*(WALLPG/1000.)
      KWN=KWHUSE-KWHR
      POWERC=KWN*CPOWER
      IF(ITER.LE.IPR)
     1WRITE(6,19)MWU,KWHUSE,MWT,KWHR,MWN,KWN
   19 FORMAT(10X,'ELECTRIC POWER REQUIREMENTS:',/,
     110X,'POWER CONSUMED',T40,-0PF8.3,' MW OR ',T64,0PE10.3,' KWHR',/,
     *10X,'TURBINE OUTPUT',T39,'-',-0PF8.3,' MW OR ',T64,0PE10.3,' KWHR'
     *,//,10X,'TOTAL',T40,-0PF8.3,' MW OR ',T64,0PE10.3,' KWHR',//)
C    LABOR COSTS
C     FRINGE BENEFITS
      FRINGE=SALTOT*FPCT
      CSALT1=FRINGE+SALTOT
C    CONTINGENCY ON LABOR
      CONLAB=CLPCT*CSALT1
      CLABOR=CONLAB+CSALT1
C   REPLACEMENT COSTS
C    OPTICAL UNITS
      COPTIC=1.5*(OPRATE*COUNIT)
C    COLLECTOR UNITS
      CRFURB=1.3*(CLRATE*CLUNIT)
C    OTHER WORK MATERIALS
      CAWM=0.07*1.2*CSALT1
C   TOTAL REPLACEMENT COSTS
      CREPL=CAWM+CRFURB+COPTIC
C   MAINTAINENCE COSTS
C    E-O SYSTEM
      COLP=OCPWAT*WAITAV
C    OTHER MAINT. COSTS
      COPM=1.E5*(MOFLOW/MOFLWB)
C   TOTAL MAINT. COSTS
      CMAINT=COPM+COLP
C   UTILITY COSTS
C    ELECTRIC POWER
C      SEE ABOVE
C    COOLING WATER
      CCW=(KWCAP/KWCAPB)*AVAIL*2500.*1.13E4*(30./1.E6)
C    PLANT AIR
      CAIR=25.E3*(MOFLOW/MOFLWB)
C    OTHER UTILITIES
      COTHL=15.E3*(ATOT/ATOTB)
C    TOTAL UTILITIES
      CUTIL=POWERC+CSTMT+CCW+CAIR+COTHL
C   INTEREST ON WORKING CAPITAL
      CIOWC=0.1*(2./12.)*(CLABOR+CREPL+CMAINT+CUTIL)
C    SUBTOTAL
```

```
      CAN1T=(CLABOR+CREPL+CMAINT+CUTIL+CIOWC)
      CANAD=(FOCG-1.)*CAN1T
      CAN1=CAN1T+CANAD
C   AMORTIZATION
      CAPCOS=CTOT
      CAMORT=CAPREC*CAPCOS
C   TOTAL ANNUAL COSTS
      ANCOST=CAMORT+CAN1
C   COST PER MOLE OF PHOTONS
      CPHOT=(CAPREC*CLRCC+0.5*FOCG*(CLABOR+COPTIC+COLP)+MWL*1000.*
     *8760.*
     1CPOWER)/MOPHOT
C   PHOTON COST PER EV-MOLE
      CEVPH=CPHOT/EVPHOT
C   PHOTON COST PER MOLE OF S REMOVED
      CPHMS=CPHOT*MOPHOT/(MOSULF*FPD)
C   COST OF GAS HANDLING($/G-MOLE OF H2S PROCESSED)
      COGH=(CGH*CAPREC+0.5*FOCG*(CLABOR+CRFURB+COPM)-(MWT-(MWU-MWL))
     **8760.*
     11000.*CPOWER+CSTMT)/(MFSULF*FPD)
      CSULF=ANCOST/(KGSULF*FPD)
      CGAS=ANCOST/((SCF/1000.)*FPD)
C     METHANOL PRODUCTION COSTS
C     SYNGAS COMPONENT
      CTONSY=CSYNGS*1.E-6*10096.*2000.
      CKGSY=(CTONSY/2000.)*2.205
C     COST OF CLAUS PLANT
      CLAUST=0.05*CTONSY
      CLAUSK=0.05*CKGSY
C     COST OF METHANOL SYNTHESIS PLANT
      CMEPT=COPME/(HRLYO*8000.)
      CMEPK=(CMEPT/2000.)*2.205
C     COST OF LASER S REMOVAL
      CLAST=ANCOST/(((CH3OH*2.205)/2000.)*FPD)
      CUNIT=ANCOST/(CH3OH*FPD)
C     TOTALS
      TON=CTONSY+CLAUST+CMEPT+CLAST
      METHC=CKGSY+CLAUSK+CMEPK+CUNIT
C     TOTAL MEOH COST W/O LASER S PROCESSING
      TONWO=TON-CLAST
      PERCT=((TON/TONWO)-1.)*100.
C     COST PER MM BTU IF MEOH IS BURNED
      CBURN=TON*1.E6/(2000.*9546.)
      IF(ITER.LE.IPR)
     1WRITE(6,1)FEEDRQ,CH3OH,METHC,TON,DAILY,HRLY,HRLYO
    1 FORMAT('0   ECONOMIC DATA:',/,' MMKG OF SYNGAS FEED= ',-6PF9.3,6X,
     1'MILLION   KG OF METHANOL PRODUCT= ',-6PF9.3,/,'   METHANOL CURREN
     2T COST = $',0PF5.3,'PER KG OR $',0PF8.1,' PER TON    @ '
     3,0PF8.2,' TONS/DAY',/,'    ',0PF8.2,'  TONS OF SYNGAS/HR DECONTAMIN
     4ATED (DESIGN BASIS)',/,'    ',0PF8.2,'  TONS OF
     5SYNGAS/HR DECONTAMINATED (ACTUAL OPERATING)',//)
```

```
      IF(ITER.LE.IPR)
     1WRITE(6,706)
  706 FORMAT(10X,'* * * TOTAL ANNUAL OPERATING COSTS IN THOUSANDS OF
     1DOLLARS * * *',//)
      IF(ITER.LE.IPR)
     1WRITE(6,707)NSTAFF,SALTOT,FPCT,FRINGE,CSALT1,CLPCT,CONLAB,
     1CLABOR,OPRATE,COUNIT,COPTIC,CLRATE,CLUNIT,CRFURB,CAWM,CREPL,OCPWAT
     2,COLP,COPM,CMAINT,CPOWER,POWERC,CSTMT,CCW,CAIR,COTHL,CUTIL,CIOWC,
     3CAN1T,FOCG,CANAD,CAN1,CAPCOS,CAPREC,CAMORT,ANCOST
  707 FORMAT(10X,'LABOR COSTS:',/,13X,'TOTAL DIRECT LABOR COSTS FOR
     1 A STAFF OF ',I2,T60,-3PF9.3,/,13X,'FRINGE BENEFITS AT ',2PF5.1,
     2' %',T60,-3PF9.3,/,T60,'----------',/,13X,'SUBTOTAL',T60,-3PF9.3,/,
     313X,'CONTINGENCY AT ',2PF5.1,' %',T60,-3PF9.3,/,T60,'----------
     4----------',/,13X,'TOTAL LABOR COSTS:',T70,-3PF9.3,//,
     510X,'REPLACEMENT & MATERIAL COSTS:',/,13X,0PF5.0,' OPTICAL
     6UNITS @ $ '0PF6.0,' @ (INCL 50% )',T60,-3PF9.3,/,
     713X,0PF5.0,' COLLECTOR UNITS @ $ ',0PF6.0,' @ (INCL 30%
     8)',T60,-3PF9.3,/,13X,'ADDITIONAL WORK MATLS(INCL 20% CONTIN
     9GENCY)',T60,-3PF9.3,/,T60,'----------',/,13X,
     *'TOTAL REPLAC. &MATERIAL
     * COSTS',T70,-3PF9.3,//,10X,'MAINTENANCE COSTS:',/,13X,'LASERS (
     *AT $',0PF5.0,' PER WATT-YR)',T60,-3PF9.3,/,13X,'OTHER PLANT
     * MAINTENANCE',T60,-3PF9.3,/,T60,'----------',/,
     *13X,'TOTAL MAINTENANCE COSTS:',T70,-3PF9.3,//,10X,'UTILITY CO
     *STS:',/,13X,'ELECTRIC POWER AT ',0PF5.2,' PER KW-HR',T60,
     *-3PF9.3,/,13X,'STEAM',T60,-3PF9.3,/,13X,'COOLING WATER',T60,-3PF
     *9.3,/,13X,'PLANT AIR',T60,-3PF9.3,/,13X,'OTHER  UTILITIES',T60,
     *-3PF9.3,/,T60,'----------',/,T13,'TOTAL UTILITY COST',
     *T70,-3PF9.3,//,10X,'INTEREST ON WORKING CAPITAL',T70,-3PF9.3,
     */,T70,'----------',/,10X,'SUBTOTAL ANNUAL COSTS',T69,-3PF10.3,//,
     *10X,'ADDTL O.C. DUE TO FOCG=  ',0PF5.3,T69,-3PF10.3,/,
     *T70,'----------',/,10X,'ADJUSTED OPERATING COSTS',
     *T69,-3PF10.3,//
     *10X,'AMORTIZATION OF CAPITAL',/,10X,'($',0PF12.0,' AT CAPITAL
     * RECOVERY OF ',0PF7.4,')',T70,-3PF9.3,/,T70,'----------',/,
     *10X,'TOTAL ANNUAL COSTS',T70,-3PF9.3,///)
      IF(ITER.LE.IPR)
     1WRITE(6,4)CPHOT,CEVPH,CPHMS,COGH,CUNIT,PERCT
    4 FORMAT('0  UNIT COSTS:',/,'  $/MOLE OF PHOTONS',T50,F7.3,
     *T60,'*',/,'  $/EV-MOLE OF PHOTONS',T50,F7.3,T60,'*',/
     *,'  PHOTON COST PER MOLE OF S REMOVED',T50,F7.3,T60,'**',/
     *,'  $/MOLE H2S IN FEED(GAS HANDLING)',T50,F7.3,T60,'**',/
     1,'   ADDITIONAL $/KG METHANOL PRODUCED',T50,F7.3,T60,'**',/
     2,'   PERCENT ADDITIONAL COST',T50,F7.2,T60,'**',///)
      IF(ITER.LE.IPR)
     1WRITE(6,7) CSULF,SCUT,CGAS
    7 FORMAT('   $/KG OF SULFUR REMOVED',T50,F9.3,/
     1,'   AT A STAGE CUT OF',T50,F7.3,/
     2'   $/THOUSAND SCF OF SYNGAS IRRADIATED= ',F10.3,//)
      IF(ITER.LE.IPR)
```

```
     1WRITE(6,1111)CSYNGS,CTONSY,CKGSY,COPME,CMEPT,CMEPK,CLAUST,
     1CLAUSK,CLAST,CUNIT,TON,METHC,CBURN
1111 FORMAT(35X,'CALCULATION OF METHANOL COST',//,
     *T60,'$/TON MEOH',T80,'$/KG MEOH',/,5X,'2:1 SYNGAS (300 BTU
     1/SCF @ $',F7.2,' PER MM BTU)',T60,F9.2,T80,F9.3,/,5X,'METHANOL PLT
     2 (EXCL.CLAUS PLANT & ZNO S REMOVAL',/,15X,'@ ANNUAL COST $',E9.2,
     3' /YR)',T60,F9.2,T80,F9.3,/,5X,'CLAUS HIGH CONC S REMOVAL PLANT'
     4,/,15X,'(5% OF SYNGAS COST)',T60,F9.2,T80,F9.3,/,5X,'LASER H2S REM
     5OV.**',T60,F9.2,T80,F9.3,/,T60,'----------',T80,'----------',/,5X,
     6'TOTAL COSTS',T60,F9.2,T80,F9.3,///,5X,'COST PER MILLION BTU IF
     7 METHANOL IS BURNED:  $ ',F7.2,///)
      IF(ITER.LE.IPR) WRITE(6,1116)
1116 FORMAT(10X,'*   INCLUDES EFFECTS OF FCOG,FOOG,FPDF',/,
     *10X,'**  INCLUDES EFFECTS OF FCOG,FOOG,FPFD,&FPD',//)
      IF (ITER.LE.IPR) WRITE(6,1117) FPD,FCOG,FOOG,FPDF
1117 FORMAT('   FIGURE OF MERIT ADJUSTMENT FACTORS',//,
     *7X,'PERFORMANCE DISCOUNT FACTOR:',T45,F7.3,/
     *7X,'CAPITAL COST GROWTH FACTOR:',T45,F7.3,/
     *7X,'OPERATING COST GROWTH FACTOR:',T45,F7.3,/
     *7X,'PROJECT DELAY PENALTY FACTOR:',T45,F7.3,///)
      RETURN
      END
```

APPENDIX K

OUTPUT OF SYNGAS CLEANUP ASSESSMENT MODEL FOR BASELINE PROCESS

INPUT DATA

FDRQKG=	.604E+09
SIGMA=	.100E-16
TEMP=	273.0
TORR=	760.0
PPMH2S=	5.0
FRMACH=	1.00
HIZ=	1.00
WIZ=	2.00
PCOLLF=	1.0
COLLIF=	12.0
RECRAT=	0.30E-10
COUNIT=	800.
CCPWAT=	500.
OCPWAT=	100.
EFF=	0.0100
FPD=	1.000
FCCG=	1.000
FOCG=	1.000
FPDF=	1.000

* * R.A.M. ANALYSIS & PLANT AVAILABILITY CALCULATION * *

LASER SYSTEM:OPTICS MTBF OF 57.4 HR & MTTR OF 0.50 HR
GIVES AVAILABILITY OF: 0.99136
MS COLLECTOR:COLL MTBF OF 12.0 HR & MTTR OF 0.25 HR
GIVES AVAILABILITY OF: 0.97959
COMPRESSORS:SINGLE COMP; 0.99900 ; 4 COM 0.99601
TURBINES:SINGLE TURBINE; 0.99500 ; 3 TUR 0.98507
NOZZLE: 0.99300
UTILITIES & SUPPORT: 0.99900
OPERATIONAL AVAILABILITY: 0.98700

TOTAL PLANT AVAILABILITY: 0.93291

SYNGAS DATA:
FEEDLB= 1.427E+09 LB/YR FEEDKG= 6.472E+08 KG/YR
VOLUMETRIC FLOWRATE(CM3SC)= 4.312E+07 CM3/SEC AT A DENSITY OF
2.689E+19 MOLECULES/CM3
TEMP= 273. K PRESSURE= 760. TORR SONIC VELOCITY= 54707. CM/SEC
GAS VELOCITY IS 1.0000 OF SONIC OR 54706.775CM/SEC VOLUME FLOW IS 4.802E+10 SCF/YR
AVE SYNGAS MOL.WT. = 10.667 H2 TO CO RATIO IN FEED= 2.0

TO OBTAIN POWER RECOVERY FOR POST PHOTOLYSIS RECOMPRESSION
THREE TURBINES ARE USED TO REDUCE PRESSURE FROM GASIFIER AT 31.6 ATM DOWN TO 1.90 ATM
AT NOZZLE PLENUM.IN EACH TURBINE THE TEMPERATURE FALLS FROM 579.6 R TO 442.1 R
THUS REQUIRING 0.126E+12 BTU/YR OF REHEAT PER TURBINE OR A TOTAL OF 0.378E+12 BTU/YR
THE TOTAL TURBINE WORK AVAILABLE IS 0.378E+12 BTU/YR OR 16969.2 HP

FOUR OR MORE COMPRESSORS ARE REQUIRED TO RECOMPRESS 91367.0 SCFM
OF SYNGAS FROM THE COLLECTION ZONE PRESSURE OF 1.00 ATM BACK INTO
THE METHANOL SYNTHESIZER AT 76.00 ATM. INPUT GAS TEMPERATURE IS 491.0 R

COMPR. #	SUCTION VOL. (CFM)	OUTPUT T (F)	REQD COOLING (BTU/YR)	POWER (HP)	COST ($MM)
	0.0	31.0	0.00E+00	0.0	0.
1	79865.4	277.0	0.20E+12	8994.8	2098154.
2	28052.7	295.0	0.22E+12	9593.8	1249045.
3	9384.2	295.0	0.22E+12	9593.8	799501.
4	3494.1	299.0	0.22E+12	9753.6	560645.
			0.85E+12	37936.1	4707345.

HEAT EXCHANGE AND ENERGY REQUIREMENTS

***TOTAL COMPRESSOR POWER:	37936.1 HP
(24023.0 KW ELECT. EQUIV.)	
HEAT PRODUCED BY STEAM TURBINE DRIVEN COMP.:(BTU/YR)	0.851E+12
PORTION USED TO PARTIALLY REHEAT SYNGAS(LAST COMP)	0.219E+12
PORTION WHICH MUST BE REMOVED BY HEAT EXCHANGERS	0.632E+12
LB OF COOLANT PER HOUR REQUIRED	0.100E+07
TOTAL HEAT EXCHR TUBE AREA REQD(FT2)	2966.
HOURLY HEAT EXCHANGER LOAD(BTU/HR)	0.722E+08
STEAM REQT FOR COMPRESSORS(LB/YR @600PSIA,1000F)	0.216E+10
REFRIGERATION LOAD TO RECOOL COMPRESSOR COOLANT(TONS)	3340.

***TOTAL POWER PRODUCED BY EXPANSION TURBINE 16969. HP OR 10746.KW

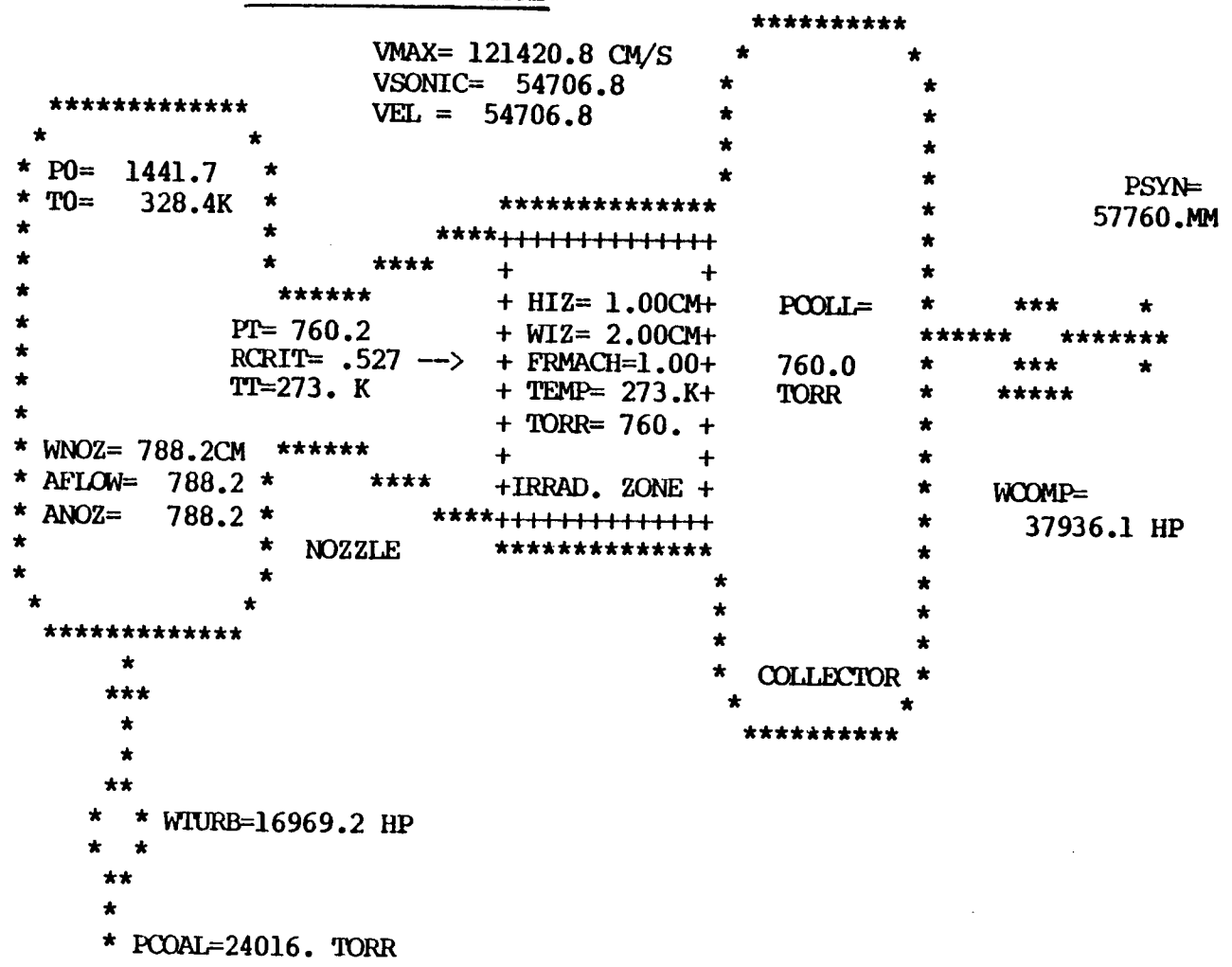
REHEAT REQTS FOR EACH OF THREE TURBINES	0.126E+12
LB OF HEAT TRANSFER FLUID PER HOUR(ALL TURBINES)	0.135E+07
HEAT EXCHR TUBE AREA PER TURBINE REHEATER(FT2)	685.
HOURLY HEAT EXCHANGER LOAD PER TURBINE(BTU/HR)	0.144E+08

***POST COMPRESSION REHEAT OF SYNTHESIS GAS FROM 299. TO 448. F

STEAM REQUIREMENT(LB/YR : 600PSIA,1000F)	0.126E+09
HEAT EXCHANGER AREA REQUIRED(FT2)	128.
HOURLY HEAT EXCHANGER LOAD(BTU/HR)	0.156E+08

***ELECTRIC POWER USE-COOLANT PUMPS & REFRIGERATION:
TOTAL CENTRIFUGAL PUMP CAPACITY OF 0.471E+04GPM REQUIRES
HYDRAULIC HP OF 59.418 OR 46.596 KW ELECTRIC.
CHILLER/REFRIG FOR COMPRESSOR COOLANT REQUIRES 3089.788 HP OR 2423.045 KW

NOZZLE CALCULATIONS



IRRADIATION ZONE DATA:

IRRADIATION ZONE HT= 1.000 CM IRRADIATION ZONE WIDTH= 2.000 CM
IRR ZN XSECT AREA= 2.0000 CM2
FLOW AREA THROUGH IRR ZONE= 788.214 CM2 NOZZLE LENGTH= 788.2 CM
IRR ZONE VOL = 1576.43 CM3
TRANSIT TIME PAST IRRAD.ZONE WIDTH= .00004 SEC LASER BEAM PATH LENGTH THRU GAS= 788.2 CM
LASER BEAM FRESNEL NUMBER = 60.41 DIFFRACTION LIMITED
PATH LENGTH(FRESNEL # OF 0.8) = 59523.8

* * * MATL BALANCES FOR DESIRED SULFUR REMOVAL * * *

STAGE S CUT OF 0.980000 REQD FOR A DF OF 50.00

	KG/YR	WT.FRACT S	LB-M/YR	M/O S
F	.64722337E+09	0.00001500	.13374877E+09	0.00000500
P	.64721386E+09	0.00000030	.13379121E+09	0.00000010
W(S)	.95142347E+04	1.00000000	.65536897E+03	1.00000000

* * * PROCESS QUANTUM YIELD AND PHOTOLYTIC CUT REQTS FOR DESIRED SULFUR REMOVAL * * *

AVERAGE HS FRAGMENT COLLISIONAL DATA:

COLL X-SECT= 3.5E-08 CM2 MOLEC SPEED= 4.19E+04CM/SEC
MEAN FREE PATH= 1.367E+00 CM COLL/SEC= 3.06E+04 COLL/(CM3*SEC)= 2.06E+18
TIME BETWEEN COLLISIONS= 3.27E-05

```
REQD QUANTUM YIELD TO GET DESIRED CUT    0.989950
REQD TRANSIT TIME(SEC) TO COLLECTOR POR .503E-05
REQD PORE DIAMETER TO CAPTURE HS (CM)      0.2107
EST COLLISIONAL MEAN FREE PATH OF HS FR    1.3669
EST REQD PHOTOLYTIC CUT                  0.989950
EST PHOTON FLUX REQD(PHOTONS/CM2-SEC)    .460E+18
EST LASER FLUENCE REQD(J/CM2)              0.435


 REQTS TO REDUCE S CONC FROM   5.0 PPM  TO    0.1 PPM
STAGE S CUT (BY WEIGHT) =   0.980000
STAGE S CUT (BY MOLAR VOL.) =   0.980000
QUANTUM YIELD EST FOR POST PHOTOLYSIS EFFECTS =      0.9899
REQD SULFUR PHOTOLYTIC CUT =   0.989950
REQD LASER FLUENCE TO REACH ABOVE AS LIMITING CUT=   0.44  φo

  OPTIMIZATION
  ITERA=  2   THSTG=   0.97258651  QY=   0.99012595  THAVE=   0.98228564
    .
    .
    .                                                  θ
                                                        ave
  ITERA=  7   THSTG=   0.97967362  QY=   0.99005401  THAVE=   0.98951533

  * * * ACTUAL POST-PHOTOLYSIS MATERIAL BALANCES * * *
  FINAL
  ITERA=  7   THSTG=   0.98069898  QY=   0.99004360  THAVE=   0.99056140

H2S DATA:
  H2S CONC. IN SYNGAS=    5. PPM       NUMBER DENSITY=   1.344E+14 MOLECULES/CM3
 MOLECULES H2S/SEC=   5.794E+21      G-MOLES OF S REMOVED/YR=   297530.29
  KG S REMOVED=     9520.97       LB S REMOVED/YR=   20993.74     H2S PART PRESS=   3.800E-03 TORR
  G-MOLES OF S IN FEED/YR=   303385.95      PPM H2S IN CLEAN SYNGAS=      0.10
```

PHOTOLYSIS & E-O DATA:

LAMBDA= 210.0 PHFLUX = 5.2E+17 PHIUV= 0.495 SIGMA= 1.0E-17
NH2S= 1.3E+14 K=1.34E-03 ENSIGW=1.06E+00
THLIM= .994668E+00 THETA= .984770E+00 THAVE= .990561E+00 WNOZ= 788.2
PUTIL= 0.20054 PULSE=1.00E-07 REP=2.74E+04 EFF=1.000E-02 WATTI=9.907E+06
WATTAV=2.710E+04 WALLPG= 2.71E+06 MOLES OF PHOTONS/YR= 1.50E+06
N*SIGMA*L FOR SYNGAS= 1.70E-01 RATIO OF H2S ABS TO CO ABS= 6.25E+00
LASER PULSE ENERGY = 0.991 JOULES

****POST-PHOTOLYSIS EFFECTS****

AVERAGE SYNTHESIS GAS COLLISIONAL DATA:

COLL X-SECT= 3.0E-08 CM2 MOLEC SPEED= 7.36E+04CM/SEC
MEAN FREE PATH= 9.303E-06 CM COLL/SEC= 7.91E+09 COLL/(CM3*SEC)= 1.06E+29
TIME BETWEEN COLLISIONS= 1.26E-10

AVERAGE HS FRAGMENT COLLISIONAL DATA:

COLL X-SECT= 3.5E-08 CM2 MOLEC SPEED= 4.19E+04CM/SEC
MEAN FREE PATH= 1.380E+00 CM COLL/SEC= 3.03E+04 COLL/(CM3*SEC)= 2.02E+18
TIME BETWEEN COLLISIONS= 3.30E-05

HS FRAGMENT RECOMBINATION DATA:
KINETIC RATECONSTANT= 3.0E-11 CM3/(MOLECULE*SEC) T 1/2 = 2.503E-04 SEC
COLLECTOR TUBE DIAM.= 0.211 CM HS TRANSIT TO WALL= 5.03E-06 SEC QUANTUM YIELD= 0.990

FINAL MATERIAL BALANCE

	KG/YR	WT.FRACT S	LB-M/YR	M/O S
F	.64722337E+09	0.00001500	.13374877E+09	0.00000500
P	.64721385E+09	0.00000029	.13345124E+09	0.00000010
W(S)	.95209694E+04	1.00000000	.65605430E+03	1.00000000

VOLUMETRIC DECONTAMINATION FACTOR: 51.93
REACTIVITY IN G-MOLES/CM3/SEC: .5984E-05

LASER SYSTEM DESIGN

IF A SINGLE LASER HEAD IS LIMITED TO A
PRF OF 1.250 KHZ, THE SYSTEM PRF OF 27.353
KHZ REQUIRES 22 LASER SETS AT AN OUTPUT POWER OF
1.238KW EACH.

A SINGLE LASER HEAD IS LIMITED TO AN OUTPUT POWER OF 7.500 KW
THE NUMBER OF LASER HEADS PER LASER SET IS 1 AT 1.238 KW PER HEAD.
THE TOTAL NUMBER OF HEADS IN THE LASER SYSTEM IS 22

* * * PLANT AREA ESTIMATES * * *	
PLENUM, IRRADIATION ZONE, COLLECTOR	1543.
EXPANSION TURBINES & REHEATERS &GENERATOR	3800.
COMPRESSORS, COOLERS, &MOTORS	4200.
LASER SYSTEM, INCL. POWER CONDITIONING	880.
BEAM HANDLING EQPT	440.
COLLECTOR REFURBISHMENT	2500.
SYNGAS STORAGE TANKS	1200.
PROCESS SUPPORT	1250.
TOTAL ADD-ON BLDG AREA (FT2)	15813.

* * ELECTRIC POWER CONSUMPTION & PRODUCTION IN KW * *	
LASERS	2710.02
CENTRIFUGAL COOLANT PUMPS	46.60
REFRIGERATION	2423.04
INSTR.&CONTROLS	100.00
LIGHTING	28.82
HEATING & VENTILATION	139.50
RECIRC. WATER SYSTEM	782.65
TOTAL OPERATING POWER CONSUMED	6230.63
ELECT PROD FROM TURBINES	10745.76
NET POWER USE OR PRODUCTION	4515.14
TOTAL INSTALLED CAPACITY (POWER CONSUMING HARDWARE ONLY)	6852.03

* * * PLANT CAPITAL COST ESTIMATE * * THOUSANDS OF $

NOZZLE,PLENUM,DISCH.SECT.&INIT.COLL.	157.643
SPARE COLLECTOR UNITS	8.011
LASER SYSTEM	13550.089
BEAM TRANSPORT SYSTEM	2710.018
OPTICAL MULTIPLEXER	100.000
SPARE OPTICAL UNITS	4.000
EXPANSION TURBINES	649.499
TURBINE REHEATERS	70.047
TURBINE GENERATORS	405.937
COMPRESSORS	4707.345
COMPRESSOR STEAM TURBINES	1400.415
COMPRESSOR COOLERS	94.931
REFRIGERATION FOR COMPRESSOR COOLANT	552.639
HEAT EXCHR. FOR POST COMP.REHEAT	5.811
STORAGE TANK FOR PLENUM SYNGAS	233.682
HEAT EXCHANGER COOLANT PUMPS	87.944
COOLING WATER SYSTEM FOR LASERS	162.682
INSTRUMENTATION AND CONTROL	100.000
PRE-OPERATIONAL CHECKOUT	115.411
OUTSIDE UTILITIES(INCL. SWITCHGEAR)	2289.286
SPECIAL SHOPS(INCL.COLL.REFAB)	50.005
ELECTRICAL DISTRIBUTION SYSTEM	40.006
SYSTEM PIPING	17.337
BUILDING	1897.563
SUBTOTAL	29410.300
ENGINEERING AT 25.000 % OF DIRECT COSTS	7352.575
SUBTOTAL	36762.875
CONTINGENCY AT 41.307 % OF ABOVE	15185.560
SUBTOTAL	51948.435
INTEREST DURING CONSTRUCTION AT 10.000 %	5194.843
ADDTL IDC DUE TO FPDF OF 1.000	0.000
TOTAL CAPITAL COST	57143.278
ADDTL CAP COST DUE TO FCCG OF 1.000	0.000
TOTAL ADJUSTED CAPITAL COST	57143.278

* * * STAFFING TABLE &COSTS FOR 5 SHIFT OPERATION * * *

CATEGORY	# OF EMPLOYEES (M)	(WT)	(WC)	(H)	LABOR COST ($ THOUSANDS)
SUPERVISORY	5				170.000
E-O SYSTEM REPAIR & COLLECTOR REFURB				15	300.000
TECHNICAL SUPPORT		1			22.000
CLERICAL SUPPORT			1		14.000
TOTAL COST FOR A STAFF OF	22				492.000

UTILITIES

STEAM REQTS & ANNUAL COSTS AT 2.90 PER THOUSAND LB:		
STEAM TURBINE DRIVEN COMPRESSORS:	0.216E+10 LB/YR	6273.87
REHEAT OF SYNGAS PRIOR TO MEOH REACTOR:	0.126E+09 LB/YR	365.06
TOTAL STEAM COST		6638.93

ELECTRIC POWER REQUIREMENTS:			
POWER CONSUMED	6.231 MW OR		0.546E+08 KWHR
TURBINE OUTPUT	- 10.746 MW OR		0.941E+08 KWHR
TOTAL	-4.515 MW OR		-0.396E+08 KWHR

ECONOMIC DATA:

MMKG OF SYNGAS FEED= 603.800 MILLION KG OF METHANOL PRODUCT= 603.800

METHANOL CURRENT COST = $ .221PER KG OR $ 200.8 PER TON @ 1823.81 TONS/DAY

81.46 TONS OF SYNGAS/HR DECONTAMINATED (DESIGN BASIS)

75.99 TONS OF SYNGAS/HR DECONTAMINATED (ACTUAL OPERATING)

* * * TOTAL ANNUAL OPERATING COSTS IN THOUSANDS OF DOLLARS * * *

LABOR COSTS:		
TOTAL DIRECT LABOR COSTS FOR A STAFF OF 22	492.000	
FRINGE BENEFITS AT 25.0 %	123.000	
SUBTOTAL	615.000	
CONTINGENCY AT 20.0 %	123.000	
TOTAL LABOR COSTS:		738.000
REPLACEMENT & MATERIAL COSTS:		
142. OPTICAL UNITS @ $ 800. @ (INCL 50%)	170.969	
681. COLLECTOR UNITS @ $ 801. @ (INCL 30%)	709.253	
ADDITIONAL WORK MATLS(INCL 20% CONTINGENCY)	51.660	
TOTAL REPLAC. &MATERIAL COSTS		931.882
MAINTENANCE COSTS:		
LASERS (AT $ 100. PER WATT-YR)	2710.018	
OTHER PLANT MAINTENANCE	99.999	
TOTAL MAINTENANCE COSTS:		2810.017
UTILITY COSTS:		
ELECTRIC POWER AT 0.03 PER KW-HR	-1186.578	
STEAM	6638.930	
COOLING WATER	0.791	
PLANT AIR	25.000	
OTHER UTILITIES	14.375	
TOTAL UTILITY COST		5492.519
INTEREST ON WORKING CAPITAL		166.207
SUBTOTAL ANNUAL COSTS		10138.625
ADDTL O.C. DUE TO FOCG= 1.000		0.000
ADJUSTED OPERATING COSTS		10138.625
AMORTIZATION OF CAPITAL ($ 57143278. AT CAPITAL RECOVERY OF 0.1102)		6297.189
TOTAL ANNUAL COSTS		16435.814

OTHER FIGURES OF MERIT

UNIT COSTS:	
$/MOLE OF PHOTONS	3.460
$/EV-MOLE OF PHOTONS	0.586
PHOTON COST PER MOLE OF S REMOVED	17.436
$/MOLE H2S IN FEED(GAS HANDLING)	22.846
ADDITIONAL $/KG METHANOL PRODUCED	0.027
PERCENT ADDITIONAL COST	14.02

$/KG OF SULFUR REMOVED		1726.275
AT A STAGE CUT OF		0.981
$/THOUSAND SCF OF SYNGAS IRRADIATED=	0.342	

CALCULATION OF METHANOL COST

	$/TON MEOH	$/KG MEOH
2:1 SYNGAS (300 BTU/SCF @ $ 7.20 PER MM BTU)	145.38	0.160
METHANOL PLT (EXCL.CLAUS PLANT & ZNO S REMOVAL @ ANNUAL COST $ 0.14E+08 /YR)	23.44	0.026
CLAUS HIGH CONC S REMOVAL PLANT (5% OF SYNGAS COST)	7.27	0.008
LASER H2S REMOV.**	24.69	0.027
TOTAL COSTS	200.78	0.221

COST PER MILLION BTU IF METHANOL IS BURNED: $ 10.52

MVSS DATA FOR SYNGAS CLEANUP ASSESSMENT MODEL

```
1917   500SYNGAS CLEANUP
 0FDRQKG   0.6038E+9
-4SIGMA    .7500E-17 .1000E-17 .5000E-16
-1TEMP    273.      250.      400.
-1TORR    760.      100.      1520.
 0PPMH2S  5.
-1FRMCH   1.        .9        1.8
-1HIZ     1.        .5        2.
 0WIZ     2.
-1PCOLLF  1.        .2        1.2
-1COLLIF  12.       8.         20.
-1RECRAT   .3000E-10 .1000E-10 .5000E-10
-1COUNIT  2000.     1000.     3000.
-1CCPWAT  500.      300.      800.
-1OCPWAT  100.      50.       200.
-1EFF     .01       .005      .025
 0FPD     1.
 0FCCG    1.
 0FOCG    1.
 0FPDF    1.
   PUTIL   PHIUV     MWN  WATTAV   AVAIL     CGH   CLRCC     CTOT  ANCOST  CPHOT
    COGH   CUNIT   STAFF   PERCT   COSTT   PATHL     TON
```

APPENDIX L

INPUT INSTRUCTIONS FOR THE MONTE CARLO DRIVER CODE

The model or models undergoing simulation must constitute or be called by a subroutine entitled FUNCT, which is itself called by the Monte Carlo driver MAIN. Transfer of information between the MAIN and FUNCT (and any other subroutines called by FUNCT) is facilitated by a common block of 45 variables[1] entitled /WHY/. In the MAIN, /WHY/ is dimensioned Y(45). In FUNCT and other subroutines, /WHY/ consists of the input variables and output figures of merit to be handled by the driver. This is best shown by an example.

Given the following subroutine FUNCT and a figure of merit, Q, depending on several variables,

```
      SUBROUTINE FUNCT
      COMMON/WHY/ A,B,C,D,Q,Y(40)
      COMMON/PRINT/ ITER,INTER,IPR
      Q=A*B+C/D
      IF(ITER.LE.IPR) WRITE(6,1) Q
    1 FORMAT('    Q=',F8.2,/)
      RETURN
      END
```

A, B, C, and D are the uncertainty inputs and will have their ranges and distribution defined. Q is the figure of merit for which an output distribution is desired. Y(40) fills in the unused space in COMMON/WHY/. The sum of the number of input and figure-of-merit (output) variables must be 45 or less. The COMMON block /PRINT/ supplies print control, and

---

[1]In recent versions of this code 100 variable capability has been added.

by setting IPR* equal to the number of iterations for which printout is desired (if any), one can reduce the amount of printout produced. ITER designates the number of Monte Carlo iterations and is supplied in the data below. All WRITE statements in the program should be preceded by IF(ITER.LE.IPR)...

The input data and specification of distribution is handled as follows. The data can be punched on cards or submitted as a data file on a terminal.

Line or Card 1:

Columns 1-2	Integer number of input variables (NVAR)
Columns 3-4	Integer number of output variables (NOUT) (NVAR + NOUT ≤ 45)
Columns 5-10	Integer number of iterations (right justified) (ITER) (ITER ≤ 999,999). (-) sign before ITER supresses printout of input distributions
Columns 11-50	Title or commentary, such as case number

For each of the NVAR input variables, the following line (or lines in the case of the histogram) provides data on the input range and type of distribution to be used. An example input data set is shown in Table L.1 and is utilized in an example below.

---

*IPR is defined in the Monte Carlo driven MAIN. INTER is also defined in the MAIN, and by setting INTER = i, every ith iteration will be printed out, e.g. INTER = 10, the ITER = 10, 20, 30,... etc. will be printed.

Table L.1

Sample Input Data

```
0901  2000EXAMPLE CASE: 2000 ITERATIONS
-1X1        200.      100.      500.
 0X2        50.
 1X3
6.          6.        1.
-2X4        100.      8.
-3X5        100.      8.        120.
-4X6        1.        0.5       2.
-6X7        5.        7.        10.       11.
-5X8        10.       0.2
 5X9
5.          5.        0.1       0.2       0.4       0.2       0.1
YY
```

Seven types of distributions are capable of definition with only a single line of data. They are shown in the accompanying Table L.2. The first two columns on the card or line supply the variable JTYPE, which defines the distribution. On columns 3-10 is entered the FORTRAN name of the input variable. Columns 11-20, 21-30, and 31-40 define the needed numerical parameters, one or more, of the PDF distribution, Z_1, Z_2, Z_3, and Z_4, respectively. The table also designates the nature of the values to be supplied for each distribution. The Z_1 through Z_4 are supplied in F or right justified E format.

For the histogram distribution, JTYPE, in columns 1 and 2, is a positive integer which defines the number of equally spaced bins which define the histogram. Columns 3-10 again supply the variable name. Additional lines supply the following information in 8F10.0 FORMAT.

Columns 1-10 Minimum [lower bound of first interval $(\Delta Z)_1$]

Columns 11-20 Size of intervals, ΔZ

Columns 21-30,

31-40, etc. Probability value corresponding to each interval $(\Delta Z)_i$. The sum of all $(\Delta Z)_i$ must equal 1.0

Final Card: The last card supplies the names of the output variables in 10A8 format. The following example illustrates correct input format.

Consider a simulation for the following relationship in FUNCT:

Y = Y (X1, X2, X3, X4, X5, X6, X7, X8, X9)

where the distributions shown on Figure L.1 are specified (the input data for these is in Table L.1).

Table L.2

Defining Parameters for Non-Histogram Input Distributions

Type of Distribution	JTYPE	Z1	Z2	Z3	Z4
Constant	0	Value	--	--	--
Triangle	-1	Mode	Min	Max	--
Normal	-2	Mean	σ	--	--
Normal with Upper Limit	-3	Mean	σ	Max	--
Log-Transformed Triangle	-4	Mode (=Median)	Min	Max	--
Log-Transformed Normal	-5	Mean	S-Parameter	--	--
Trapezoid	-6	Min	Vertex-1	Vertex-2	Max

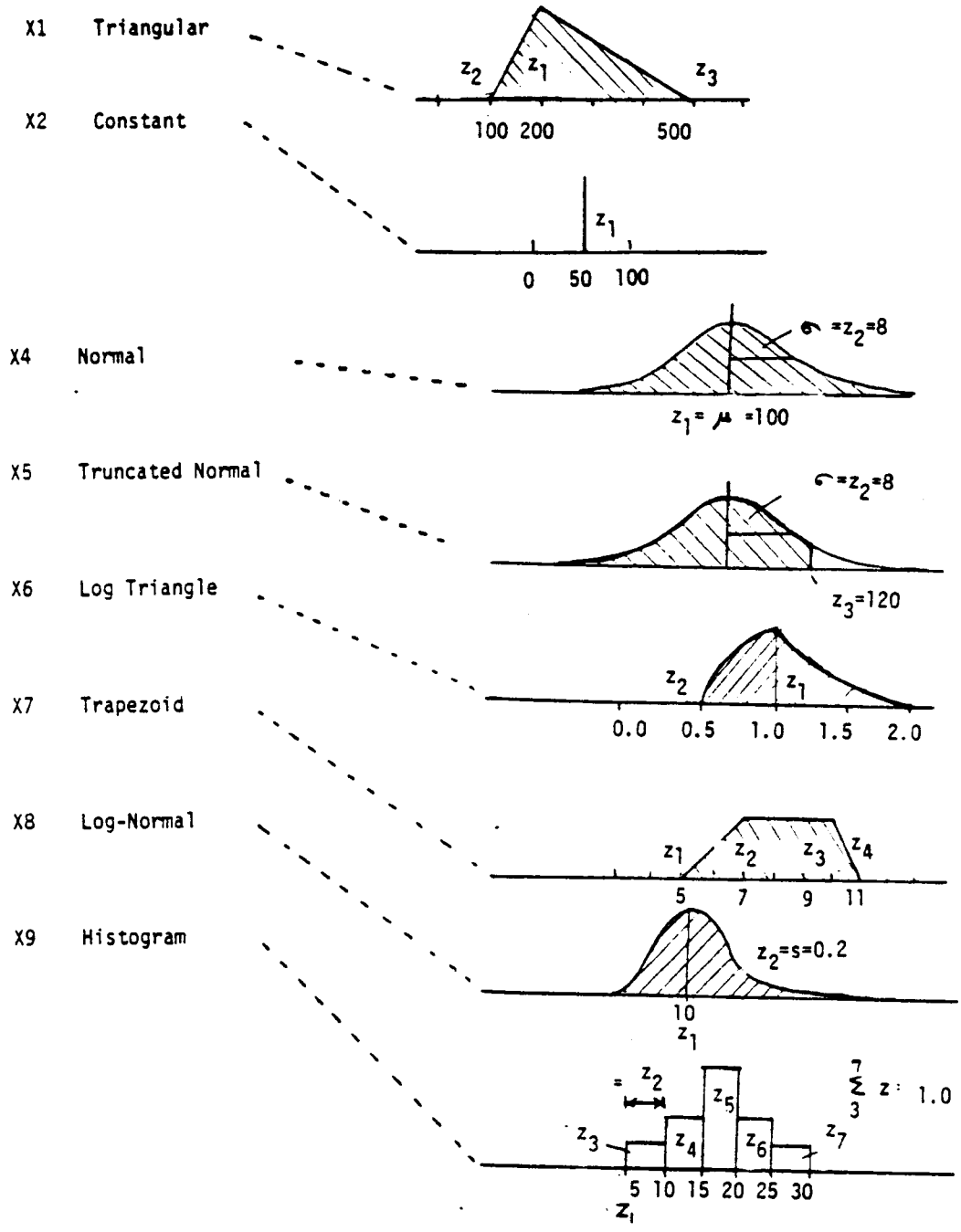


Figure L.1

Available Distributions

An example SUBROUTINE FUNCT which supplies the function $Y = Y(X_i)$ is shown in Fig. L.2.

```
      SUBROUTINE FUNCT
      COMMON/WHY/X1,X2,X3,X4,X5,X6,X7,X8,X9,YY,Y(35)
      COMMON/PRINT/ITER,INTER,IPR
      YY=X1/X3+X2+X4+((X7*X8)**X6)/(X5*X9)
      IF (ITER.LE.IPR) WRITE(6,1)ITER,X1,X2,X3,X4,X5,X6,X7,X8,X9,YY
    1 FORMAT(' ',I4,3X,9(F7.3,2X),5X,F10.3/)
      RETURN
      END
```

Figure L.2

Example SUBROUTINE FUNCT

The actual X_i input distributions and the resulting output distribution on Y for a 2000 iteration simulation are shown in Figs. L.3 and L.4.

MONTE CARLO UNCERTAINTY ANALYSIS FOR EXAMPLE CASE: 2000 ITERATIONS
DATE: TIME: 09:41

9 INPUT VARIABLES 1 OUTPUT VARIABLES 2000 ITERATIONS
28 STORAGE LOCATIONS USED FOR INPUT DATA

SUMMARY OF INPUT DATA

I	NAME	DIST	DATA						
1	X1	TRIANGLE	200.0	100.0	500.0				
2	X2	CONSTANT	50.00						
3	X3	HISTOGRM	6.000	6.000	1.000				
4	X4	NORMAL	100.0	8.000					
5	X5	NORMAL.	100.0	8.000	120.0				
6	X6	LOG-TRI	1.000	0.5000	2.000				
7	X7	TRAPZOID	5.000	7.000	10.00	11.00			
8	X8	LOG-NORM	10.00	0.2000					
9	X9	HISTOGRM	5.000	5.000	0.1000	0.3000	0.7000	0.9000	1.000

Figure L.3

Sample Input Data and Input Histograms

STATISTICS FOR INPUT VARIABLE X1 (TRIANGLE DISTRIBUTION)

MINIMUM 101.59 MAXIMUM 495.93

MEAN 264.71 VARIANCE 7110.3 STD.DEVIATION 84.323

PERCENTILES: 2.5% 128. 5.0% 143. 50.0% 253. 95.0% 421. 97.5% 445.

2000 POINT HISTOGRAM * = 3 POINTS

PROB	CUME	VALUE		
0.0135	0.0000	100.0	27	*********
0.0295	0.0135	120.0	59	**********
0.0490	0.0430	140.0	98	**********
0.0670	0.0920	160.0	134	**********
0.0930	0.1590	180.0	186	**********
0.0920	0.2520	200.0	184	**********
0.0960	0.3440	220.0	192	**********
0.0915	0.4400	240.0	183	**********
0.0760	0.5315	260.0	152	**********
0.0775	0.6075	280.0	155	**********
0.0605	0.6850	300.0	121	**********
0.0455	0.7455	320.0	91	**********
0.0490	0.7910	340.0	98	**********
0.0430	0.8400	360.0	86	**********
0.0295	0.8830	380.0	59	**********
0.0360	0.9125	400.0	72	**********
0.0220	0.9485	420.0	44	**********
0.0185	0.9705	440.0	37	**********
0.0075	0.9890	460.0	15	*****
0.0035	0.9965	480.0	7	**
	1.0000	500.0		

Figure L.3 (Continued)

(X_2 IS A CONSTANT: NO DISTRIBUTION SHOWN)

STATISTICS FOR INPUT VARIABLE X3 (UNIFORM DIST.)

MINIMUM 6.0017 MAXIMUM 11.999

MEAN 9.0184 VARIANCE 2.9835 STD.DEVIATION 1.7273

PERCENTILES: 2.5% 6.15 5.0% 6.30 50.0% 9.03 95.0% 11.7 97.5% 11.8

2000 POINT HISTOGRAM * = 6 POINTS

PROB	CUME	VALUE		
0.1975	0.0000	6.000	395	**********
0.2060	0.1975	7.200	412	**********
0.1825	0.4035	8.400	365	**********
0.2205	0.5860	9.600	441	**********
0.1935	0.8065	10.80	387	**********
	1.0000	12.00		

Figure L.3 (Continued)

STATISTICS FOR INPUT VARIABLE X4 (NORMAL DISTRIBUTION)

MINIMUM 71.112 MAXIMUM 128.90

MEAN 99.908 VARIANCE 61.876 STD.DEVIATION 7.8662

PERCENTILES: 2.5% 84.7 5.0% 87.1 50.0% 100. 95.0% 113. 97.5% 115.

2000 POINT HISTOGRAM * = 3 POINTS

PROB	CUME	VALUE		
0.0005	0.0000	70.00	1	
0.0000	0.0005	72.00	0	
0.0010	0.0005	74.00	2	*
0.0005	0.0015	76.00	1	
0.0040	0.0020	78.00	8	***
0.0055	0.0060	80.00	11	****
0.0080	0.0115	82.00	16	*****
0.0160	0.0195	84.00	32	**********
0.0265	0.0355	86.00	53	**********
0.0430	0.0620	88.00	86	**********
0.0520	0.1050	90.00	104	**********
0.0740	0.1570	92.00	148	**********
0.0815	0.2310	94.00	163	**********
0.0880	0.3125	96.00	176	**********
0.1015	0.4005	98.00	203	**********
0.1030	0.5020	100.0	206	**********
0.0965	0.6050	102.0	193	**********
0.0855	0.7015	104.0	171	**********
0.0595	0.7870	106.0	119	**********
0.0545	0.8465	108.0	109	**********
0.0360	0.9010	110.0	72	**********
0.0275	0.9370	112.0	55	**********
0.0165	0.9645	114.0	33	**********
0.0090	0.9810	116.0	18	******
0.0040	0.9900	118.0	8	***
0.0020	0.9940	120.0	4	*
0.0030	0.9960	122.0	6	**
0.0005	0.9990	124.0	1	
0.0000	0.9995	126.0	0	
0.0005	0.9995	128.0	1	
	1.0000	130.0		

Figure L.3 (Continued)

STATISTICS FOR INPUT VARIABLE X5 (NORMAL DISTRIBUTION WITH TRUNCATED RIGHT TAIL)

MINIMUM 77.655 MAXIMUM 120.00

MEAN 100.03 VARIANCE 61.591 STD.DEVIATION 7.8480

PERCENTILES: 2.5% 84.4 5.0% 86.8 50.0% 100. 95.0% 113. 97.5% 116.

2000 POINT HISTOGRAM * = 3 POINTS

PROB	CUME	VALUE		
0.0010	0.0000	76.00	2	*
0.0030	0.0010	78.00	6	**
0.0070	0.0040	80.00	14	*****
0.0105	0.0110	82.00	21	*******
0.0165	0.0215	84.00	33	**********
0.0300	0.0380	86.00	60	**********
0.0350	0.0680	88.00	70	**********
0.0525	0.1030	90.00	105	**********
0.0725	0.1555	92.00	145	**********
0.0815	0.2280	94.00	163	**********
0.0885	0.3095	96.00	177	**********
0.0960	0.3980	98.00	192	**********
0.0910	0.4940	100.0	182	**********
0.1060	0.5850	102.0	212	**********
0.0820	0.6910	104.0	164	**********
0.0795	0.7730	106.0	159	**********
0.0475	0.8525	108.0	95	**********
0.0355	0.9000	110.0	71	**********
0.0230	0.9355	112.0	46	**********
0.0180	0.9585	114.0	36	**********
0.0115	0.9765	116.0	23	**********
0.0070	0.9880	118.0	14	**********
0.0050	0.9950	120.0	10	**********
	1.0000	122.0		

Figure L.3 (Continued)

STATISTICS FOR INPUT VARIABLE X6 (LOG TRIANGLE DISTRIBUTION)

MINIMUM 0.50630 MAXIMUM 1.9439

MEAN 1.0430 VARIANCE 9.08403E-02 STD.DEVIATION 0.30140

PERCENTILES: 2.5% .581 5.0% .617 50.0% 1.00 95.0% 1.62 97.5% 1.73

2000 POINT HISTOGRAM * = 2 POINTS

PROB	CUME	VALUE		
0.0090	0.0000	0.5000	18	*********
0.0260	0.0090	0.5500	52	**************************
0.0430	0.0350	0.6000	86	***
0.0440	0.0780	0.6500	88	**
0.0545	0.1220	0.7000	109	***
0.0605	0.1765	0.7500	121	**
0.0600	0.2370	0.8000	120	**
0.0580	0.2970	0.8500	116	**
0.0685	0.3550	0.9000	137	**
0.0745	0.4235	0.9500	149	**
0.0705	0.4980	1.000	141	**
0.0545	0.5685	1.050	109	***
0.0605	0.6230	1.100	121	**
0.0400	0.6835	1.150	80	**
0.0435	0.7235	1.200	87	***
0.0380	0.7670	1.250	76	**************************************
0.0270	0.8050	1.300	54	***************************
0.0290	0.8320	1.350	58	*****************************
0.0235	0.8610	1.400	47	************************
0.0300	0.8845	1.450	60	******************************
0.0185	0.9145	1.500	37	*******************
0.0125	0.9330	1.550	25	************
0.0120	0.9455	1.600	24	************
0.0120	0.9575	1.650	24	************
0.0080	0.9695	1.700	16	********
0.0075	0.9775	1.750	15	********
0.0055	0.9850	1.800	11	******
0.0060	0.9905	1.850	12	******
0.0035	0.9965	1.900	7	****
	1.0000	1.950		

Figure L.3 (Continued)

STATISTICS FOR INPUT VARIABLE X7 (TRAPEZOIDAL DISTRIBUTION)

MINIMUM 5.2117 MAXIMUM 10.840

MEAN 8.2782 VARIANCE 1.8666 STD.DEVIATION 1.3662

PERCENTILES: 2.5% 5.70 5.0% 5.95 50.0% 8.33 95.0% 10.3 97.5% 10.5

2000 POINT HISTOGRAM * = 2 POINTS

PROB	CUME	VALUE		
0.0045	0.0000	5.200	9	*****
0.0125	0.0045	5.400	25	**********
0.0160	0.0170	5.600	32	**********
0.0230	0.0330	5.800	46	**********
0.0260	0.0560	6.000	52	**********
0.0195	0.0820	6.200	39	**********
0.0250	0.1015	6.400	50	**********
0.0345	0.1265	6.600	69	**********
0.0400	0.1610	6.800	80	**********
0.0480	0.2010	7.000	96	**********
0.0475	0.2490	7.200	95	**********
0.0495	0.2965	7.400	99	**********
0.0415	0.3460	7.600	83	**********
0.0420	0.3875	7.800	84	**********
0.0415	0.4295	8.000	83	**********
0.0455	0.4710	8.200	91	**********
0.0395	0.5165	8.400	79	**********
0.0410	0.5560	8.600	82	**********
0.0490	0.5970	8.800	98	**********
0.0520	0.6460	9.000	104	**********
0.0545	0.6980	9.200	109	**********
0.0325	0.7525	9.400	65	**********
0.0485	0.7850	9.600	97	**********
0.0505	0.8335	9.800	101	**********
0.0440	0.8840	10.00	88	**********
0.0325	0.9280	10.20	65	**********
0.0255	0.9605	10.40	51	**********
0.0125	0.9860	10.60	25	**********
0.0015	0.9985	10.80	3	**
	1.0000	11.00		

Figure L.3 (Continued)

STATISTICS FOR INPUT VARIABLE X8 (LOG NORMAL DISTRIBUTION)

MINIMUM 5.2294 MAXIMUM 18.280

MEAN 10.167 VARIANCE 4.1888 STD.DEVIATION 2.0467

PERCENTILES: 2.5% 6.64 5.0% 7.06 50.0% 9.95 95.0% 13.9 97.5% 14.9

2000 POINT HISTOGRAM * = 4 POINTS

PROB	CUME	VALUE		
0.0005	0.0000	5.000	1	
0.0050	0.0005	5.500	10	***
0.0115	0.0055	6.000	23	******
0.0280	0.0170	6.500	56	***************
0.0390	0.0450	7.000	78	********************
0.0575	0.0840	7.500	115	******************************
0.0745	0.1415	8.000	149	**************************************
0.0810	0.2160	8.500	162	**
0.0935	0.2970	9.000	187	**
0.1210	0.3905	9.500	242	**
0.1000	0.5115	10.00	200	**
0.0780	0.6115	10.50	156	**
0.0780	0.6895	11.00	156	**
0.0565	0.7675	11.50	113	******************************
0.0445	0.8240	12.00	89	***********************
0.0370	0.8685	12.50	74	*******************
0.0290	0.9055	13.00	58	***************
0.0200	0.9345	13.50	40	**********
0.0090	0.9545	14.00	18	*****
0.0130	0.9635	14.50	26	*******
0.0120	0.9765	15.00	24	******
0.0055	0.9885	15.50	11	***
0.0020	0.9940	16.00	4	*
0.0025	0.9960	16.50	5	*
0.0005	0.9985	17.00	1	
0.0005	0.9990	17.50	1	
0.0005	0.9995	18.00	1	
	1.0000	18.50		

Figure L.3 (Continued)

STATISTICS FOR INPUT VARIABLE X9 (4 BOX HISTOGRAM DISTRIBUTION)

MINIMUM 5.0050 MAXIMUM 29.936

MEAN 17.574 VARIANCE 32.921 STD.DEVIATION 5.7377

PERCENTILES: 2.5% 6.20 5.0% 7.40 50.0% 17.6 95.0% 27.6 97.5% 28.8

2000 POINT HISTOGRAM * = 6 POINTS

PROB	CUME	VALUE		
0.0520	0.0000	5.000	104	**********
0.0520	0.0520	7.500	104	**********
0.0920	0.1040	10.00	184	**********
0.0980	0.1960	12.50	196	**********
0.1980	0.2940	15.00	396	**********
0.2070	0.4920	17.50	414	**********
0.0950	0.6990	20.00	190	**********
0.0990	0.7940	22.50	198	**********
0.0555	0.8930	25.00	111	**********
0.0515	0.9485	27.50	103	**********
	1.0000	30.00		

Figure L.3 (Continued)

STATISTICS FOR OUTPUT VARIABLE YY

MINIMUM 144.32 MAXIMUM 230.62

MEAN 180.58 VARIANCE 204.90 STD.DEVIATION 14.314

PERCENTILES: 2.5% 156. 5.0% 159. 50.0% 179. 95.0% 207. 97.5% 214.

2000 POINT HISTOGRAM * = 4 POINTS

PROB	CUME	VALUE		
0.0005	0.0000	140.0	1	
0.0020	0.0005	145.0	4	*
0.0155	0.0025	150.0	31	********
0.0380	0.0180	155.0	76	********************
0.0690	0.0560	160.0	138	************************************
0.1180	0.1250	165.0	236	**
0.1360	0.2430	170.0	272	**
0.1385	0.3790	175.0	277	**
0.1290	0.5175	180.0	258	***
0.1190	0.6465	185.0	238	***
0.0830	0.7655	190.0	166	**
0.0595	0.8485	195.0	119	******************************
0.0320	0.9080	200.0	64	****************
0.0235	0.9400	205.0	47	************
0.0145	0.9635	210.0	29	*******
0.0110	0.9780	215.0	22	******
0.0070	0.9890	220.0	14	****
0.0030	0.9960	225.0	6	**
0.0010	0.9990	230.0	2	*
	1.0000	235.0		

Figure L.4

Example Output Histogram for Function YY

APPENDIX M

FORTRAN LISTING OF MONTE CARLO DRIVER CODE

```
      REAL*8 NAME
      REAL LOW,IN
      LOGICAL ZOUT
      COMMON /QZQ/ NAME(45),INDEX,NVAR,NK,NITER,LTYPE(2,44),XDATA(300)
      COMMON /WHY/ Y(45) ---------- TRANSFER COMMON BLOCK
      COMMON /PRINT/ ITER,INTER,IPR
      DIMENSION ZMIN(45),ZMAX(45),SUM(45),SUM2(45),NHIST(45,40)
      DIMENSION NDV(45),XLOW(45),XDIFF(45)
      DIMENSION PER(6),XPER(5)
      DATA PER/ 0.025, 0.05, 0.50, 0.95, 0.975, 2.00/
      DATA STAR,BLANK/'*',' '/
      DATA IN,OUT/'  IN',' OUT'/
C  MAXIMUM NSMAX IS 75
      DATA NSMAX/75/
      INT(X)=INT1(X)
      IPR=0
      IOUT=6
C  READ PROBABILITY DISTRIBUTIONS
      CALL READIN(ZOUT)
      CALL PRINTX
      DO 100 K=1,NK
      ZMIN(K)=1E30
      ZMAX(K)=-1E30
      SUM(K)=0.
      SUM2(K)=0.
  100 CONTINUE
C
C  BEGIN MONTE CARLO
      DO 200 ITER=1,NITER
C  SELECT RANDOM VALUES FOR EACH VARIABLE
      CALL XVALUE
C  PERFORM FUNCTION EVALUATION
      CALL FUNCT ----------> ASSESSMENT MODEL
      TYPE *,ITER
```

```
C  STORE RESULTS
       WRITE(1) (Y(K),K=1,NK)
       DO 200 K=1,NK
       ZMIN(K)=AMIN1(ZMIN(K),Y(K))
       ZMAX(K)=AMAX1(ZMAX(K),Y(K))
       SUM(K)=SUM(K)+Y(K)
       SUM2(K)=SUM2(K)+Y(K)**2
  200 CONTINUE
C  END MONTE CARLO
C
C  ANALYZE RESULTS
C  SET HISTOGRAM INTERVALS
       DO 250 K=1,NK
       NDES=40
       IF(K.GT.NVAR) GO TO 210
       JTYPE=LTYPE(1,K)
       IF(JTYPE.LE.0.OR.JTYPE.GT.NDES) GO TO 210
C  HISTOGRAM DISTRIBUTIONS--USE SAME INTERVALS AS INPUT
       ISTART=LTYPE(2,K)
       XLOW(K)=XDATA(ISTART)
       NDV(K)=JTYPE
       IF(JTYPE.LT.10) NDV(K)=JTYPE*2
       IF(JTYPE.LT.5) NDV(K)=JTYPE*5
       XDIFF(K)=XDATA(ISTART+1)*JTYPE/NDV(K)
       GO TO 250
  210 CONTINUE
C  THIS SECTION FOR OTHER DISTRIBUTIONS
       YMIN=ZMIN(K)
       YMAX=ZMAX(K)
       IF(K.GT.NVAR) YMAX=AMIN1(YMAX,YMIN+4.*(SUM(K)/NITER-YMIN))
       IF(YMAX.LE.YMIN) YMIN=0.
       IF(YMAX.LE.YMIN) YMAX=1.
       LHI=ALOG10(YMAX-YMIN)+100.
       DIFF=10.**(LHI-101)/2.
       NDIV=INT(YMAX/DIFF)-INT(YMIN/DIFF)+1
       M=1
       IF(NDIV.GT.NDES) M=2
```

```
      IF(NDIV+1.GT.NDES*2) M=4
      IF(NDIV+3.GT.NDES*4) M=10
      DIFF=DIFF*M
      NDIV=INT(YMAX/DIFF)-INT(YMIN/DIFF) + 1
      LOW=INT(YMIN/DIFF)*DIFF
      XLOW(K)=LOW
      NDV(K)=NDIV
      XDIFF(K)=DIFF
  250 CONTINUE
C  PUT NUMBERS IN HISTOGRAM
      CALL ZERO(NHIST(1,1),NDES*4*45)
      REWIND 1
      DO 300 I=1,NITER
      READ (1) (Y(K),K=1,NK)
      DO 300 K=1,NK
      J=(Y(K)-XLOW(K)) / XDIFF(K) + 1.
      IF(J.GT.NDES) GO TO 300
      NDV(K)=MAX0(NDV(K),J)
      NHIST(K,J)=NHIST(K,J)+1
  300 CONTINUE
      REWIND 1
C  SET UP HISTOGRAMS TO BE PRINTED
      DO 500 K=1,NK
      PUT=OUT
      IF(K.GT.NVAR) GO TO 555
C  BYPASS CONSTANTS
      IF(ZOUT .OR. LTYPE(1,K).EQ.0) GO TO 500
      PUT=IN
  555 CONTINUE
      AVG=SUM(K)/NITER
      VAR=(SUM2(K)-AVG*SUM(K))/NITER
      STD=SQRT(VAR)
      WRITE(IOUT,6) PUT,NAME(K),ZMIN(K),ZMAX(K),AVG,VAR,STD
    6 FORMAT(/1H1,4X,'STATISTICS FOR',A4,'PUT VARIABLE',1X,A8/
     >       1H0,4X'MINIMUM',1PG15.5,T30,'MAXIMUM',G15.5/
     > '0',4X,'MEAN',G15.5,T30,'VARIANCE',G15.5,T55,
     > 'STD.DEVIATION',G15.5)
C  PRINT HISTOGRAM
      NDIV=NDV(K)
      DIFF=XDIFF(K)
      LOW=XLOW(K)
      NHMAX=1
      IF(NITER.LT.100) GO TO 71
      NHTOT=0
      LJK=1
      NEXT=NITER*PER(1)
      DO 70 J=1,NDIV
      NHTOT=NHTOT+NHIST(K,J)
   69 IF(NHTOT.LT.NEXT) GO TO 70
      IF(LJK.GE.6) GO TO 500
      XTOP=LOW+DIFF*J
```

```
      XPER(IJK)=XTOP-DIFF*(NHTOT-NEXT)/NHIST(K,J)
      IJK=IJK+1
      NEXT=NITER*PER(IJK)
      GO TO 69
   70 NHMAX=MAX0(NHMAX,NHIST(K,J))
      WRITE(IOUT,7) (PER(IJK),XPER(IJK),IJK=1,5)
    7 FORMAT('0    PERCENTILES: ',5(2X2PF5.1,'%',1PG9.3))
   71 NSCALE=(NHMAX+NSMAX-1)/NSMAX
      WRITE(IOUT,10) NITER,NSCALE
   10 FORMAT('0',5XI6,' POINT HISTOGRAM',10X,'* =',I3,'  POINTS'/
     > '0  PROB',6X,'CUME',8X,'VALUE'/)
      NNDIV=MIN0(NDIV,50)
      NCUME=0
      DO 400 J=1,NNDIV
      YY=LOW+DIFF*(J-1)
      N=NHIST(K,J)
      PROB=FLOAT(N)/FLOAT(NITER)
      CUME=FLOAT(NCUME)/FLOAT(NITER)
      NCUME=NCUME+N
      FIELD=BLANK
      IF(N.GE.1) FIELD=STAR
      NN=(N+NSCALE/2)/NSCALE
      WRITE(IOUT,11) PROB,CUME,YY,N,(FIELD,I=1,NN)
   11 FORMAT(1X,F7.4,F10.4,3X,1PG12.4,I5,3X75A1)
  400 CONTINUE
      HIGH=LOW+DIFF*NDIV
      CUME=FLOAT(NCUME)/FLOAT(NITER)
      WRITE(IOUT,12) CUME,HIGH
   12 FORMAT(8X,F10.4,3X,1PG12.4)
C  SAVE HISTOGRAM DATA FOR DISSPLA PLOTTING
C     IF(K.GT.NVAR)
C    > WRITE(7,72) LOW,DIFF,NDIV,NHMAX,(NHIST(K,J),J=1,NDIV)
C  72 FORMAT(1X,1P2G13.5,2I8/(1X11I6))
  500 CONTINUE
      STOP
      END
      FUNCTION INT1(X)
C  THIS FUNCTION COMPUTES THE LARGEST INTEGER THAT IS LESS THAN X.  THIS
C  DIFFERS FROM TRUNCATION FOR X.LT.0.
      INT1=X
      IF(X.GE.0.) RETURN
      I=1-INT1
      INT1=INT(X+FLOAT(I))-I
      RETURN
      END
      SUBROUTINE READIN(ZOUT)
      REAL*8 ZDATE,ZTIME
      REAL*8 XNAME,NAME
      LOGICAL ZOUT
      COMMON /QZQ/ NAME(45),INDEX,NVAR,NK,NITER,LTYPE(2,44),XDATA(300)
      DIMENSION TITLE(10)
```

```
C     CALL IDAY(ZDATE)
      CALL TIME(ZTIME)
      READ(5,90) NVAR,NOUT,NITER,TITLE
      ZOUT=NITER.LT.0
      NITER=IABS(NITER)
      WRITE(6,200) TITLE,ZDATE,ZTIME,NVAR,NOUT,NITER
      NK=NVAR+NOUT
      IF (NK.GT.45.OR.NVAR.GT.44) WRITE(6,201)
      INDEX=1
      DO 1 NUMBER=1,NVAR
      READ(5,100) JTYPE,XNAME,X1,X2,X3,X4
      NAME(NUMBER)=XNAME
      LTYPE(1,NUMBER)=JTYPE
      LTYPE(2,NUMBER)=INDEX
      IF(JTYPE.GT.0) GO TO 10
      JTYPE=-JTYPE
      XDATA(INDEX)=X1
      INDEX=INDEX+1
      IF(JTYPE.EQ.0) GO TO 1
      GO TO (3,2,3,3,2,4),JTYPE
    2 XDATA(INDEX)=X2
      INDEX=INDEX+1
      GO TO 1
    3 XDATA(INDEX)=X2
      IF (X3.EQ.0.) X3=1.
      XDATA(INDEX+1)=X3
      INDEX=INDEX+2
      GO TO 1
    4 XDATA(INDEX)=X2
      XDATA(INDEX+1)=X3
      XDATA(INDEX+2)=X4
      INDEX=INDEX+3
      GO TO 1
   10 IEND=INDEX+JTYPE+1
      READ(5,101)(XDATA(I),I=INDEX,IEND)
      ISTART=INDEX+2
      SUM=0.
      IF(XDATA(ISTART).EQ.0.) XDATA(ISTART)=1.
      DO 11 I=ISTART,IEND
      SUM=SUM+XDATA(I)
   11 XDATA(I)=SUM
      DO 12 I=ISTART,IEND
   12 XDATA(I)=XDATA(I)/SUM
      INDEX=IEND+1
    1 CONTINUE
      N1=NVAR+1
      NSTOR=INDEX-1
      WRITE(6,202) NSTOR
      READ(5,110) (NAME(I),I=N1,NK)
      RETURN
   90 FORMAT(2I2,I6,10A4)
```

```
100 FORMAT(I2,A8,4F10.0)
101 FORMAT(8F10.0)
110 FORMAT(10A8)
200 FORMAT('1 MONTE CARLO UNCERTAINTY ANALYSIS FOR ',10A4/
   > '  DATE:',1X,A8,'   TIME:',1X,A8/
   > 1H0,I4,' INPUT VARIABLES',I5,' OUTPUT VARIABLES',
   > 2X,I6,' ITERATIONS')
201 FORMAT('0>>> TOO MANY VARIABLES, PROGRAM MAY BOMB <<<'/)
202 FORMAT(5X,I5,' STORAGE LOCATIONS USED FOR INPUT DATA')
    END
```

```
    SUBROUTINE PRINTX
    REAL*8 NAME,HIST,XDIST(6),DNAME,CONST
    COMMON /QZQ/ NAME(45),INDEX,NVAR,NK,NITER,LTYPE(2,44),XDATA(300)
    DIMENSION NDIST(6)
    DATA NDIST/2,1,2,2,1,3/
    DATA HIST/'HISTOGRM'/,CONST/'CONSTANT'/
    DATA XDIST/'TRIANGLE','NORMAL','NORMAL.','LOG-TRI','LOG-NORM',
   > 'TRAPZOID'/
    WRITE(6,100)
    DO 20 I=1,NVAR
    J=LTYPE(1,I)
    ISTART=LTYPE(2,I)
    IF(J) 1,2,3
  3 DNAME=HIST
    IEND=ISTART+J+1
    GO TO 10
  2 DNAME=CONST
    IEND=ISTART
    GO TO 10
  1 DNAME=XDIST(-J)
    IEND=ISTART+NDIST(-J)
 10 CONTINUE
    WRITE(6,101) I,NAME(I),DNAME,(XDATA(K),K=ISTART,IEND)
 20 CONTINUE
    RETURN
100 FORMAT('-     SUMMARY OF INPUT DATA'/
   & '0  I  NAME      DIST          DATA'/)
101 FORMAT('0',I3,2X,A8,1X,A8,2X,(/'+',24X8G12.4))
    END
```

```
    SUBROUTINE XVALUE
    REAL*8 NAME
    COMMON /QZQ/ NAME(45),INDEX,NVAR,NK,NITER,LTYPE(2,44),XDATA(300)
    COMMON /WHY/ Y(45)
    DO 100 NUMBER=1,NVAR
    JTYPE=LTYPE(1,NUMBER)
    ISTART=LTYPE(2,NUMBER)
    Q=UNI(0)
    XMEAN=XDATA(ISTART)
    IF(JTYPE) 8,9,10
  9 X=XMEAN
    GO TO 100
```

```
    8 JTYPE=-JTYPE
      GO TO (1,2,2,4,2,6),JTYPE
C  JTYPE=2,3  NORMAL
    2 SIGMA=XDATA(ISTART+1)
      QN=RNOR(0)
      IF(JTYPE.EQ.5) GO TO 5
      QX=QN*SIGMA+XMEAN
C  SET X >= ZERO  (ACTUALLY >= XMEAN/50)
      X=AMAX1(QX,XMEAN/50.)
      IF (JTYPE.EQ.3) X=AMIN1(X,XDATA(ISTART+2))
      GO TO 100
C  LOG-NORMAL DISTRIBUTION, XMEAN IS MEDIAN
    5 X=XMEAN*EXP(QN*SIGMA)
      GO TO 100
C  JTYPE=1
C  TRIANGLE DISTRIBUTION--PDF IS ZERO AT A AND B, INCREASES LINEARLY
C  TO A MAXIMUM AT XMEAN.  INPUT VALUES ARE MODE, MIN, AND MAX.
    1 A=XMEAN-XDATA(ISTART+1)
      B=XDATA(ISTART+2)-XMEAN
      GO TO 210
C  JTYPE=4  LN(X) IS A TRIANGLE DISTRIBUTION
    4 A=-ALOG(XDATA(ISTART+1)/XMEAN)
      B=ALOG(XDATA(ISTART+2)/XMEAN)
  210 C=2./(A+B)
      D=C
      P=Q-A*C/2.
      IF (P.LT.0.) GO TO 220
      DISC=AMAX1(0.,B**2-2.*P*B/D)
      T=B-SQRT(DISC)
      GO TO 230
  220 DISC=AMAX1(0.,A**2+2.*P*A/C)
      T=-A+SQRT(DISC)
  230 IF(JTYPE.NE.4) GO TO 240
      X=XMEAN*EXP(T)
      GO TO 100
  240 X=XMEAN+T
      GO TO 100
C  JTYPE=6  TRAPEZOID
C  ZERO AT X1, RISES TO FLAT BETWEEN X2 AND X3, DROPS TO ZERO AT X4
    6 X1=XDATA(ISTART)
      X2=XDATA(ISTART+1)
      X3=XDATA(ISTART+2)
      X4=XDATA(ISTART+3)
C  FIND PROBABILITY LIMITS FOR EACH REGION
      PTOT=(X4-X1)+(X3-X2)
      P1=(X2-X1)/PTOT
      IF(Q.LT.P1) GO TO 310
      P2=1.-(X4-X3)/PTOT
      IF(Q.GT.P2) GO TO 320
C  WE'RE IN THE FLAT PART, SO INTERPOLATE
```

```
      X=X2+(Q-P1)/(P2-P1)*(X3-X2)
      GO TO 100
C  FOR TRIANGULAR REGIONS, SET UP AND USE TRIANGLE ALGORITHM
  310 A=X2-X1
      B=0.
      XMEAN=X2
      Q=Q/P1
      GO TO 210
  320 A=0.
      B=X4-X3
      XMEAN=X3
      Q=(Q-P2)/(1.-P2)
      GO TO 210
C
C  HISTOGRAM DISTRIBUTION
C  ALL VALUES EQUALLY SPACED, XMEAN IS MINIMUM VALUE
C  INPUTS ARE PROBABILITY OF EACH VALUE
C  THIS ROUTINE DOES LINEAR INTERPOLATION BETWEEN INPUT VALUES.
   10 XINCR=XDATA(ISTART+1)
      ISTART=ISTART+2
      IF(JTYPE.EQ.1) GO TO 21
      DO 20 I=2,JTYPE
      J=JTYPE-I
      IF(Q-XDATA(ISTART+J)) 20,22,22
   20 CONTINUE
   21 FUDGE=Q/XDATA(ISTART)
      J=-1
      GO TO 23
   22 FUDGE=(Q-XDATA(ISTART+J))/(XDATA(ISTART+J+1)-XDATA(ISTART+J))
   23 X=XMEAN + XINCR*(FLOAT(J+1)+FUDGE)
  100 Y(NUMBER)=X
      RETURN
      END
      FUNCTION UNI(X)
      UNI=RAN(X)
      RETURN
      END
      FUNCTION RNOR(X)
      Q=-6
      DO 100 I=1,12
  100 Q=Q+RAN(0)
      RNOR=Q
      RETURN
      END
```

UNIFORMLY DISTRIBUTED RANDOM NUMBER

LIBRARY ROUTINE ON DEC-10 COMPUTER

NORMALLY DISTRIBUTED RANDOM NUMBER

VITA

Kent Alan Williams was born in Chicago, Illinois, in 1946 and attended grade and junior high schools in LaGrange, Illinois. After receiving a diploma from Lyons Township High School in LaGrange (1964) he attended Purdue University and received a Bachelor of Science in Chemical Engineering (1968) and a Master of Science in Chemical Engineering (1970). During this period he also was a co-op student and Summer Practice School participant at the Argonne National Laboratory, a research facility of the U.S. Atomic Energy Commission.

From January 1970 to March 1984, Mr. Williams has been employed by the Operations Analysis and Planning Division of the Union Carbide Nuclear Division in Oak Ridge, Tennessee. He is presently with the same division of Martin Marietta Energy Systems, Inc., in Oak Ridge. His efforts at the UCC-ND operated Oak Ridge Gaseous Diffusion Plant have spanned many aspects of the uranium enrichment industry, with economic analysis of new enrichment technologies as his predominant interest. He spent most of 1981 in the Washington, D.C., area serving on a Department of Energy committee assembled to draft a set of criteria for selection of an advanced isotope separation technology for future U.S. uranium enrichment efforts. He has pursued further graduate education at the University of Tennessee, Knoxville since 1970, majoring in Chemical Engineering, and received his Ph.D in August 1984. He has also served in several offices, including Chairman, of the Knoxville-Oak Ridge section of the American Institute of Chemical Engineers.

Mr. Williams is married to the former Joyce Ann Soules of Gaithersburg, Maryland.