Monte Carlo Simulation as a Research Management Tool

Larry J. Douglas

June 1986

To be presented at the 1986 TAPPI
Research and Development Conference,
September 28 - October 1, 1986,
Raleigh, North Carolina

NOTICE

MONTE CARLO SIMULATION AS A
RESEARCH MANAGEMENT TOOL

Larry J. Douglas, Ph.D.
Manager, Strategic Planning
Solar Fuels Research Division
Solar Energy Research Institute
Golden, CO 80401

ABSTRACT

Monte Carlo simulation provides a research
manager with a performance monitoring tool to
supplement the standard schedule- and
resource-based tools such as the Program
Evaluation and Review Technique (PERT) and
Critical Path Method (CPM). The value of the
Monte Carlo simulation in a research environ-
ment is that it 1) provides a method for
ranking competing processes, 2) couples tech-
nical improvements to the process economics,
and 3) provides a mechanism to determine the
value of research dollars. In this paper the
Monte Carlo simulation approach is developed
and applied to the evaluation of three com-
peting processes for converting lignocellulo-
sic biomass to ethanol. The technique is
shown to be useful for ranking the processes
and illustrating the importance of the time-
frame of the analysis on the decision pro-
cess. The results show that acid hydrolysis
processes have higher potential for near-term
application (2-5 years), while the enzymatic
hydrolysis approach has an equal chance to be
competitive in the long term (beyond 10
years).

INTRODUCTION

The managers of research development in gov-
ernment and private sector organizations face
the very difficult task of selecting, from
among several potential projects, those that
most warrant funding from an ever-diminishing
research budget. Managers can use a variety
of analytical techniques to help evaluate
options and finally select the winners from
among the candidate processes. This process,
often called decision analysis, involves
development of criteria related to cost,
schedule, and performance. Gantt charts,
PERT (Program Evaluation and Review Tech-
nique) diagrams, and the CPM (Critical Path
Method) analysis are commonly used tools to
show schedule and/or cost considerations
associated with a project.(1,2) However,
they do not provide a quantitative measure of
expected performance improvement for the
programs under investigation.

The Monte Carlo simulation technique does
provide a method to couple performance with
the uncertainty in research activity. The
basic premise of the Monte Carlo technique is
that the uncertainty in a research project
can be represented by one or more random
normal distribution functions, and that if
these uncertainties are coupled to the most
sensitive activities in a project, the simu-
lation will yield the most probable results
based on the input distributions.

BACKGROUND

The Solar Energy Research Institute (SERI) is
the field manager for the Department of Ener-
gy (DOE) program to convert lignocellulosic
biomass into ethanol. There are two funda-
mental approaches to conversion, either
through acid hydrolysis of the cellulose to
glucose and subsequent fermentation to eth-
anol or through enzymatic hydrolysis of cel-
lulose and fermentation to ethanol. There
are 10 or 12 variations to these basic ap-
proaches, and SERI managers must choose the
best alternative from among these processes
for funding support and further development.

In a recent SERI study titled "Fuel Alcohol
Technical and Economic Analysis," (3) a com-
plete evaluation of the numerous process
options was conducted. Process models were
developed on a Lotus 1-2-3 spreadsheet for
each of the approaches, and subsequently used
to complete parametric and sensitivity ana-
lyses for each process. Three processes were
the most promising: the plug flow and pro-
gressing batch acid hydrolysis processes and
the separate hydrolysis and fermentation
enzymatic hydrolysis process.

OBJECTIVES

In this paper we explore the use of Monte
Carlo simulation to compare the potential of
these three processes for producing ethanol
from lignocellulosic biomass. The technical
performance improvement for each of the pro-
cesses will be evaluated by coupling the
performance changes to ethanol production
costs. As will be seen later, two equally
important considerations in ranking the pro-
cesses are the technical performance improve-
ments to each of these processes important
and the time frame in which we evaluate these
parametric improvements.

EQUIPMENT

The use of a Monte Carlo simulation requires
a computer model that gives a reasonable
representation of the process under study and
the development of a large random distribu-
tion of input data to run the model. One run
might have from 5 to 15 parameters and 250 to
1000 random numbers for each parameter. The
large number of iterations (250-1000) in-
volved in a typical Monte Carlo simulation
required the use of a main frame computer
until the advent of the desktop PC.

With a PC and a spreadsheet program, e.g.,
Lotus 1-2-3, it is now possible to complete a
Monte Carlo analysis at your desk. The Lotus

program is particularly useful for doing the simulations because of its ease of modification and debugging, built-in graphics capability, random number generator, and statistical and distribution functions. With a process simulation model developed on a Lotus spreadsheet, it is possible to complete the total Monte Carlo simulation on the same spreadsheet and display the results in graphical format.

GENERAL METHODOLOGY

The two requirements for generating useful Monte Carlo simulations are a computer model that is a reasonable representation of the process being studied, and a group of random normal distributions that reflect a reasonable expectation value for the selected parameter. The first requirement can be satisfied by evaluating the results of the model over the range of variables being used. The second requires the best judgment of experts in the technology under investigation and their concurrence with the mean values for the parameters and the expected range of each variable.

The general approach to developing and running a Monte Carlo simulation involves four steps:

● Develop a model for the process(es) in question
● Run parametric analyses with the model to determine principal areas of sensitivity
● Develop random normal distributions for each of the sensitive parameters centered about an expectation value

● Run the simulation using the selected, randomized parameters and evaluate the results.

PROCESSES EVALUATED

Cellulose is converted to ethanol by hydrolyzing the cellulose to glucose and then fermenting the glucose to ethanol. The hydrolysis step can be carried out either by an acidic medium or with enzymes. In this paper we examine two dilute-acid hydrolysis approaches and one enzymatic hydrolysis process and compare them using the Monte Carlo simulation technique.

The Plug Flow Reactor

Figure 1 is the flowsheet for the plug flow acid hydrolysis process. The plug-flow process uses dilute sulfuric acid (~1%) at high temperature and pressure, relying on a very short residence time to optimize the yield of cellulose hydrolyzed to glucose. The process uses high-pressure steam to flow a wood slurry through a "pipe" reactor at high speed. At the end of the tube the reaction is quenched; the total residence time is approximately 4 to 6 seconds. The glucose yield ranges from 50% to 60% under these conditions. The advantage of this configuration is the concurrent production of furfural from the xylose fraction of the feedstock. The favorable economics of the plug flow process rely heavily on the furfural co-product selling price.
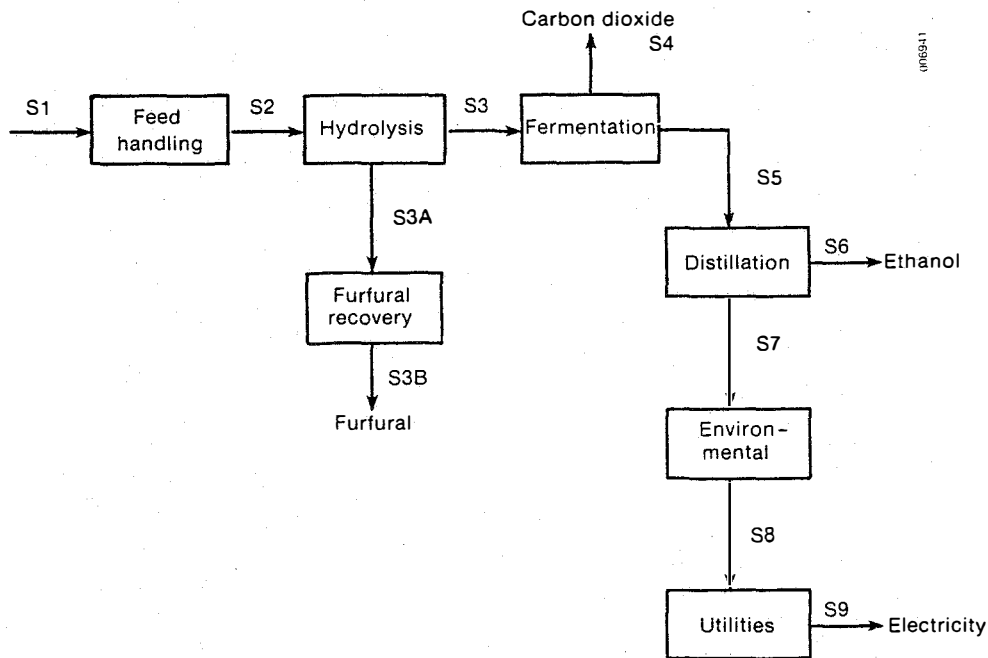

Figure 1. Acid Hydrolysis Flowsheet--Plug-Flow Reactor

The Progressing Batch Reactor

Figure 2 is the flowsheet for the progressing batch acid hydrolysis process. The progressing batch process uses dilute sulfuric acid in a multireactor adaptation of the percolation-type process, but it simulates counter-current performance. The process has two temperature zones: one at $150^{\circ}C$ to selectively remove the hemicellulose portion and a second at $180^{\circ}C$ to hydrolyze the cellulose. The residence time in this type of process is about two hours. This approach should give higher sugar yields and concentrations than the plug-flow apparatus while also reducing the degradation of both the C5 and C6 sugars.

Separate Hydrolysis and Fermentation

Figure 3 is the flowsheet for the separate hydrolysis and fermentation (SHF) process, which is the base system for enzymatic conversion of cellulose to ethanol. The process consists of specialized units to accomplish pretreatment of the feedstock, enzyme production, and hydrolysis of the cellulose to yield glucose followed by a conventional fermentation to produce ethanol. The enzymatic process has the advantage of high yields and cleaner process streams than the acid processes, but suffers from low rates of hydrolysis and enzyme production and, at present, a prohibitively high enzyme production cost.

MODELS

The models used to complete the Monte Carlo simulations were developed on a Lotus spreadsheet and were based on the models prepared in conjunction with the above-mentioned Fuel Alcohol Technology and Economic Study. The design basis for all the models was the state-of-the-art cellulose-to-ethanol plant designed by Badger Engineers (4) in 1984. The base-case plant produces 25,000,000 gallons of ethanol per year from a feedstock of mixed hardwoods. To assure the comparability of the results, all the designs were the same except the pretreatment and hydrolysis sections, which were specific to the individual processes.

From the process designs and material balances, the cost of producing ethanol is calculated. The capital costs were estimated using the ICARUS computer-aided cost estimating program. The base-case processes were developed on a Lotus 1-2-3 spreadsheet, which allowed easy parametric recalculation of the material balance. With the material balance calculated it is easy to use the spreadsheet models to calculate the electrical and thermal energy requirements of the process, the overall plant energy balance, and the plant capital cost. This information provides the basis for calculating the cost of raw materials, utilities, labor, overhead and maintenance, by-product credits, annualized capital charges, and the selling price of ethanol. These models also allow rapid calculation of sensitivities and the parametric analyses necessary to identify the parameters for inputs into the Monte Carlo simulations.

RESULTS AND DISCUSSION

With a well-developed model we can develop the input distributions for running the simulation. As an example, the economic performance of the progressing batch process was found to be very sensitive to the liquid residence time in the reactor. A consensus
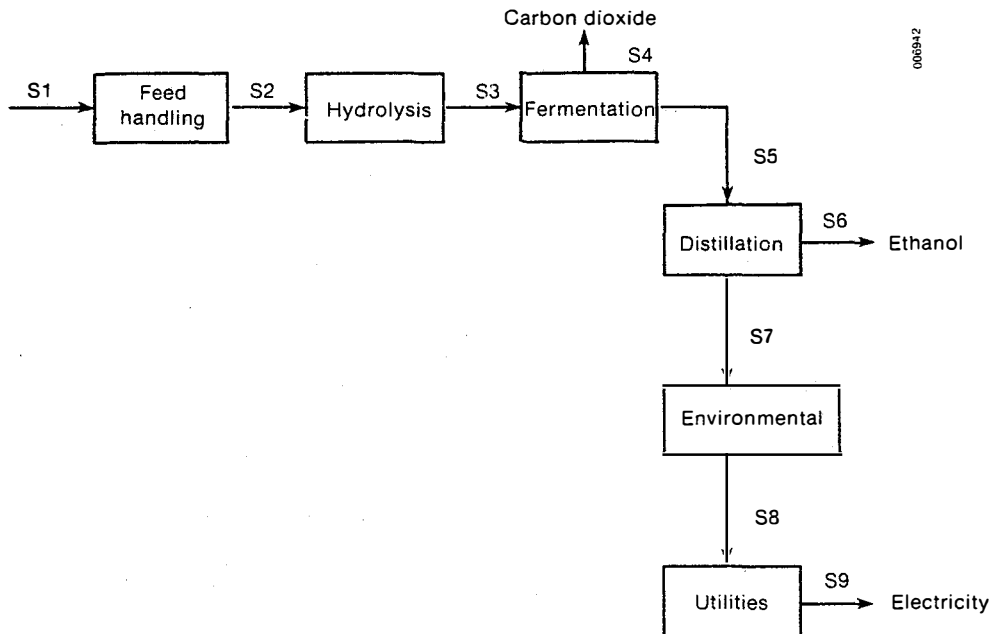

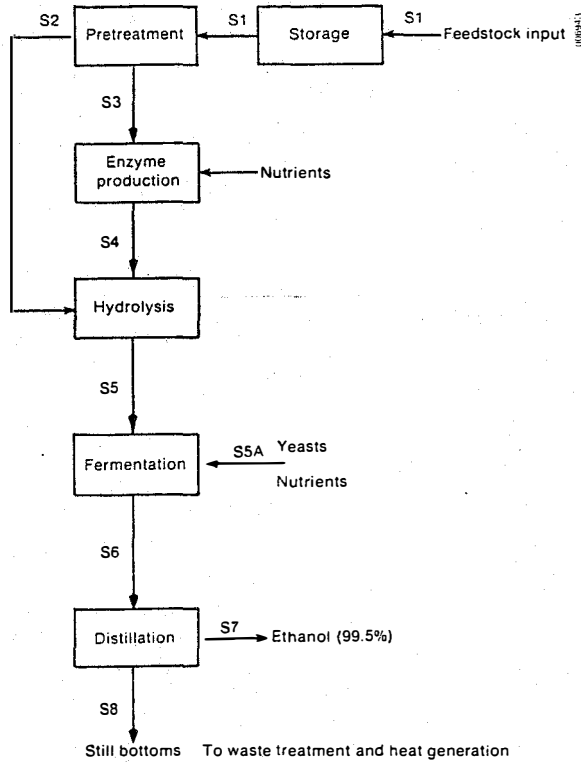Figure 2. Acid Hydrolysis Flowsheet--Progressing Batch Reactor

3

Figure 3. Separate Hydrolysis and Fermentation Flowsheet

Figure 4. Progressing Batch Acid Process 250 Point Monte Carlo Simulation

of experts in acid hydrolysis suggested a normal distribution to be generated that had a mean (expectation) value of 45 minutes and sigma (the standard deviation) of 10. This distribution contained 250 points and was used to run a Monte Carlo simulation using the Lotus 1-2-3 model for the progressing batch process, resulting in the output shown in Figure 4. Figure 4a shows the output distribution histogram for the selling price of ethanol; this curve was integrated to yield the cumulative probability curve shown in Figure 4b.(5) The 0.5 value on the probability curve corresponds to the expected selling price for ethanol resulting from this simulation.

The simulations discussed in the remainder of the paper were run using multiple variables. The variables were chosen based on the results of sensitivity analyses completed for each of the processes.

The economic performance of the plug flow dilute acid hydrolysis process was found to be very sensitive to the percent solids entering the reactor feed pump and to the assigned selling price for the furfural coproduct. The plug flow system was configured to operate using a 10% solids slurry produced ethanol at a selling price of $2.04/gallon, while a 20% solids slurry system gave ethanol at about $1.29/gallon. When the coproduct furfural selling price was set to zero the ethanol selling price was $1.99/gallon. At
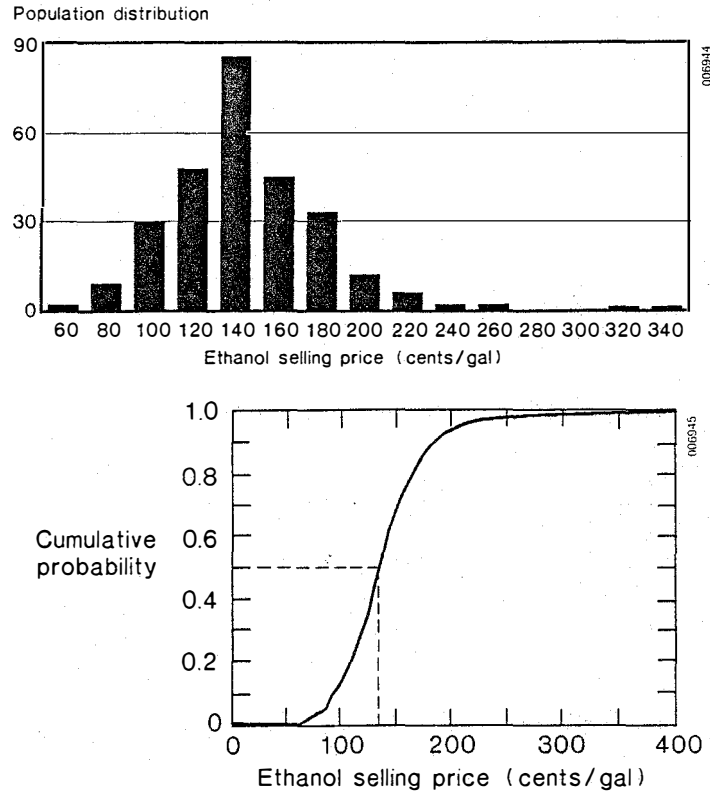
$0.12/pound for furfural credit the ethanol selling price dropped to $1.29/gallon. At 250°C the price for ethanol increased to $1.38/gallon and at 280°C the selling price dropped to $1.22/gallon. A 0.5% acid concentration in the reactor increased the selling price of ethanol to $1.32/gallon, and a 1% acid concentration in the reactor resulted in an ethanol selling price of $1.29/gallon (which is the base case).

● The plug flow simulations were run using four variables; percent solids in the reactor, by-product credit for furfural, temperature, and acid concentration.

The economic performance of the progressing batch acid hydrolysis process was also found to be sensitive to the percent solids in the reactor; e.g., at 10% solids loading in the reactor the selling price of the product ethanol was $2.02/gallon, and at 18% solids produces an ethanol selling price of $1.41/gallon. The operating temperature of the prehydrolysis and the hydrolysis reactors was found to impact the economics. With the prehydrolysis temperature increased from 150° to 165°C the ethanol selling price rose to $1.52/gallon. With the hydrolysis temperature lowered from 189° to 165°C the selling price of ethanol increased to $2.83/gallon. Reducing the liquid residence time from 45 to 25 minutes increased the ethanol selling price to $1.74/gallon. The addition of xylose fermentation to ethanol to the process

reduced the selling price of the product ethanol to $0.99/gallon. The base-case process configuration produces ethanol selling for $1.41/gallon.

● The progressing batch simulations were run using five variables: reactor packing density, prehydrolysis temperature, hydrolysis temperature in main reactor, liquid residence time, and xylose fermentation to ethanol.

The economic performance of the separate hydrolysis and fermentation enzymatic process was found to be particularly sensitive to percent solids in the hydrolysis reactor, enzyme loading in the hydrolysis step, hydrolysis time, hydrolysis yield, enzyme productivity, xylose conversion to ethanol, and lignin coproduct credit. The base-case process produced ethanol at a selling price of $2.60/gallon.

Increasing the solids loading in the hydrolysis reactor from 10% to 20% reduced the selling price of ethanol to $2.12/gallon. Reducing the enzyme loading from 20 IU/gram of solids to 7.5 IU/gram reduced the selling price of ethanol to $2.10/gallon. Reducing the hydrolysis time from 72 to 24 hours lowered the ethanol price to $2.29/gallon. Including xylose fermentation to ethanol lowered the selling price of ethanol to $1.76/gallon. Increasing the hydrolysis yield to 95% reduced the price of ethanol to $2.22/gallon. An 8X increase in the rate of enzyme production reduces the selling price of ethanol to $2.23/gallon. Separating the lignin fraction of the feedstock and realizing a net value of $0.07/pound coproduct credit reduces the ethanol selling price to $1.91/gallon.

● The separate hydrolysis and fermentation simulations were run with seven variables: percent solids in the hydrolysis reactor, enzyme loading, hydrolysis time, hydrolysis yield, xylose fermentation, enzyme productivity, and lignin by-product credit.

Figure 5 shows a comparison of the output from Monte Carlo simulations for all three processes in 1980, Figure 6 shows the same processes in 1985, and Figure 7 shows the projected comparison in 1990.

In 1980 there was no progressing batch process and little information was available on the then newly developed plug flow process. For the purposes of this report, the progressing batch process for 1980 was simulated using the standard percolation process as the basis. The difference in the expectation selling price for the two acid processes in 1980 was minimal; both would sell for about $2.35/gallon. In the same time frame the expected selling price for ethanol from the SHF process was about $6.80/gallon.

The 1985 results shown in Figure 6 demonstrate the improvement in the expectation
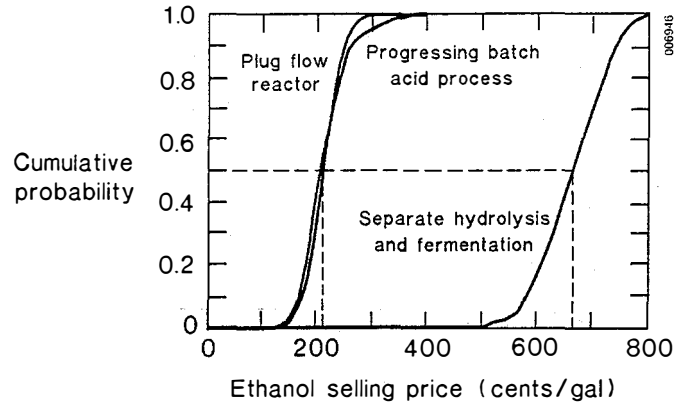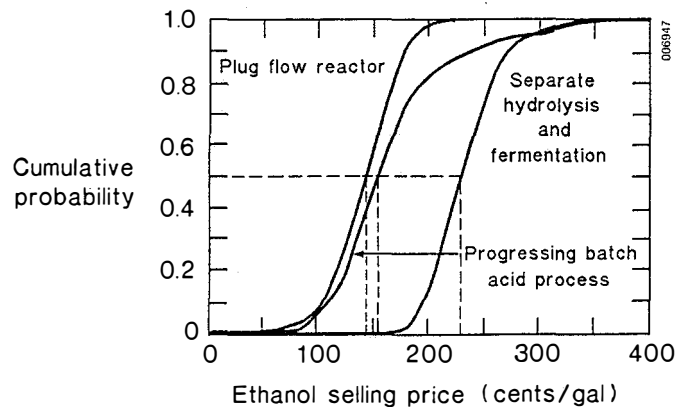

Figure 5. Monte Carlo Simulation, 1980
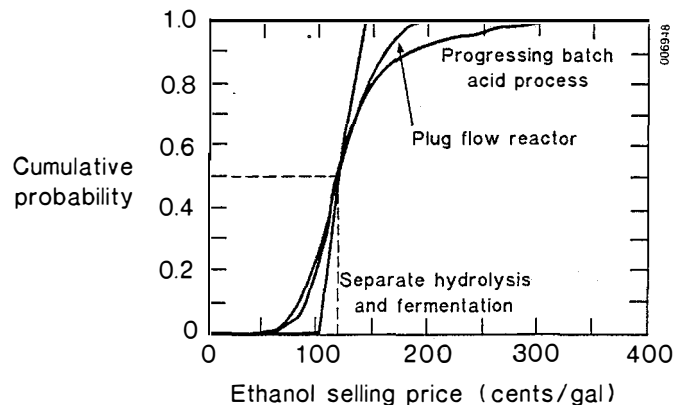

Figure 6. Monte Carlo Simulation, 1985

Figure 7. Monte Carlo Simulation, 1990

values for all three processes. The plug flow process now is at about $1.35/gallon and the progressing batch process at about $1.50/gallon. This is a significant reduction compared to the 1980 values. The SHF process shows even a more dramatic improvement, dropping from $6.80/gallon to about $2.50/gallon.

By 1990 all three processes have about the same expectation value for ethanol selling price, and any difference among the processes

will have to be evaluated outside the parameters used to complete the Monte Carlo simulations.

CONCLUSIONS

The Monte Carlo simulation technique offers the research manager a tool to monitor performance improvement and supplement the schedule and cost data generated by conventional management tools such as PERT and CPM. The value of the Monte Carlo simulation in a research environment is that it 1) provides a method for ranking competing processes, 2) couples technical improvements to the process economics, and 3) provides a mechanism to determine the value of research dollars.

The processes discussed above illustrate the use of Monte Carlo simulation that produces a result that will allow a manager to rank ethanol processes according to their ability to produce ethanol at a price competitive with alternate approaches. In addition, if the time horizon for implementation of a new process is important, the ability to have a ranking system with time attached becomes important. In the cases above, if a plant is to be constructed in the next two or three years then one of the acid hydrolysis processes would be preferred; however, if the new plant was to start after 1990 all the processes are on equal footing and other criteria would be used to differentiate among them.

Figure 8 shows the impact of changing the percent solids entering the plug flow reactor from 12% to 18%. This single change in technical performance of the hydrolysis reactor reduces the selling price of ethanol from $1.90/gallon to about $1.45/gallon. This type of analysis also helps determine the direction of future research and engineering activity. The development of a hydrolysis approach and associated reactor hardware that can handle 20% solids is our current goal for the plug flow acid hydrolysis process. The sensitivity of the process economics to this parameter is so dominating that if this ob-

jective is not met the process will cease to be competitive with the other approaches and dropped from further consideration.

In the progressing batch and separate hydrolysis and fermentation processes the economics could be greatly improved with the addition of xylose fermentation to ethanol. This step would increase the ethanol yield by as much as 50% to 70%. Figure 9 shows the impact of xylose conversion on the economics of ethanol production for the progressing batch process. If we assign a dollar figure to each of the conversion yields and assume that this curve is generated for the year 1990, then with no funding for research to improve xylose fermentation we would stay at our present position of no ethanol from xylose. Each of the higher yields represents the estimated improvement in xylose fermentation projected by technical experts based on three different budgeting scenarios: $75,000/year, $150,000/year, and $300,000/year for five years. The argument is very convincing that the resulting xylose conversion yield and impact of process economics are directly coupled to the funding level over the five years of research.

REFERENCES

1. Antunes, J., and Klopp, G., "A Method for Performance Risk Analysis," Model Simulation Processes, 10th Annual Pittsburgh Conference, 1979.
2. Muglia, V. O., "REM Management using Risk Analysis," Proceedings, 1976 Annual Reliability and Maintainability Symposium, Las Vegas, Nev., pp. 230-233.
3. Solar Energy Research Institute, Fuel Alcohol Technical and Economic Evaluation, Draft, February 1986, Golden, Colo.
4. Badger Engineers, Inc., "Economic Feasibility of an Acid-Based Ethanol Plant," Subcontract to Solar Energy Research Institute, Badger Engineers, Inc., One Broadway, Cambridge, MA 02142.
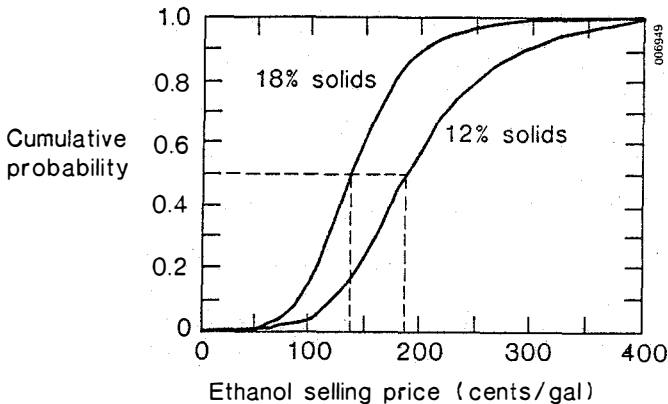5. Bury, K. V., Statistical Models in Applied Science, Chapter 2, John Wiley and Sons, 1975.

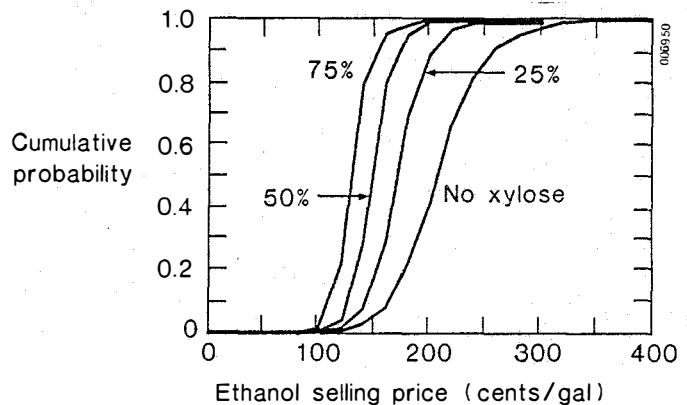Figure 8. Plug Flow Reactor 250 Point Monte Carlo Simulation

Figure 9. Xylose Fermentation Impact in Progressing Batch Reactor