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THE ECONOMICAL PRODUCTION OF ALCOHOL FUELS FROM COAL-DERIVED SYNTHESIS GAS

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Executive Summary

The preparation of candidate catalyst materials is well under way. Catalysts based on molybdenum are being prepared using four different approaches. These materials have been characterized by IR, XRD and single-crystal studies. Additional materials, of chevrel and other phases, will be prepared and characterized.

Construction of the WVU reactor units is complete. However, there have been problems with the interfacing of the reactors with the software. A computer consultant has been called in, and we anticipate being operational by the end of the next quarter. At UCC&P, the reactor units are complete. However, delays have occurred because of the retirements of key personnel and re-assignments of new personnel.

Modelling studies are continuing satisfactorily. Previous numerical results have been confirmed by using a completely different software package, geared towards solving stiff ordinary differential equations. We are seeking a more-detailed model of the reaction kinetics, to account for individual alcohols rather than a lumped higher-alcohol, to substitute into the models of the various reactors considered by us.

The overall efficiency of each base case has been calculated and tested as a screening method to select feasible technologies. This method provides similar results as the cost analysis performed earlier. However, a simple selection technique such as this fails to account for all the complex interactions of an entity like an energy park. Therefore, a more sophisticated technique is being developed to account for these factors. This method uses multiple objectives to convey these interactions.

A methodology to determine the effects and influences of process variable uncertainties on the performance of a design has been developed. Input variables in the model to be considered include the reaction product distribution, the operating temperatures of equipment (e.g., gasifiers, separators, etc.), and the estimates in the thermodynamic model used in the computer aided design simulation of the process. The efficiency of the process can be modeled by calculation of output variables such as the payback period or the energy efficiency of the plant. Determination of the parameters that may cause uncertainty in the process will be accomplished by choosing those parameters that are probabilistic in value and those which are not correlated to other more significant parameters. The result will be a range of expected operating conditions for the process and an indication of which variables' uncertainties are most likely to affect process operating conditions.

The stream exiting the reactor consists of alcohols, esters and water. The separation block consists of a network of distillation columns which separate the various alcohols and water. The streams exiting the distillation columns are rich in either one or more alcohols. The choice and order of separation, operating conditions, degree of separation and amount to be bypassed are the random variables to be optimized by simulated annealing. The value of the above variables controls the mix of the alcohol streams to be used as gasoline additives exiting the network of distillation column. The blending problem is solved as a linear program incorporating constraints on the BRVP, octane number and the amount of oxygen in each blend. The total profitability is the price obtained by selling the various blended products after accounting for the cost of production of various alcohols.

In fuels testing, the software and controls for the CFR engine were developed. The emission models that EPA has developed, the simple model and the complex model were studied, since the complex model will replace the simple model as of January 1, 1994.

TASK 1. REACTION STUDIES

1.1 Introduction

The objective of Task 1 is to prepare and evaluate catalysts and to develop efficient reactor systems for the selective conversion of hydrogen-lean synthesis gas to alcohol fuel extenders and octane enhancers.

Task 1 is subdivided into three separate subtasks: laboratory and equipment setup; catalysis research; and reaction engineering and modeling. Research at West Virginia University (WVU) is focused on molybdenum-based catalysts. Parallel research being done at Union Carbide Chemicals and Plastics (UCC&P) is focused on transition-metal-oxide catalysts.

1.2 Accomplishments, Results and Discussion

1.2.1 Laboratory Setup

At WVU, the physical construction of the reaction units is complete. The control software has been installed and programmed for the reaction unit. However, the unit and the software have not yet been interfaced. We are addressing this problem and have brought in a computer consultant to help with the interfacing problem. We expect to be operational by the end of the next quarter.

At UCC&P, the laboratory is set up for the testing of catalysts. Both Union Carbide key personnel retired during the quarter covered by this report. A new key personnel has been identified at Union Carbide. These and other personnel reassignments have hampered the progress on this project. Replacements have been named, and they are familiarizing themselves with the equipment and procedures.

1.2.2 Molybdenum-Based Catalyst Research

Approach 1. The focus of this approach is to make the organometallic products illustrated in the following five reactions:

$$Cp_2Fe_2S_2(CO)_6 + Cp_2Mo_2(CO)_4 \longrightarrow Cp_2Mo_2Fe_2S_2(CO)_8 + 2CO \tag{1}$$
$$Cp_2Mo_2(\mu\text{-}S)_2(\mu\text{-}SH)_2 + Co_2(CO)_8 \longrightarrow Cp_2Mo_2Co_2S_3(CO)_4 + 4CO \tag{2}$$
$$(Et_4N)_2M(SPh)_4 + 2Mo(CO)_4C_7H_8 \longrightarrow (NEt_4)_2\{M(SPh)_4[Mo(CO)_4]_2\} \quad (M=Co,\ Ni) \tag{3}$$
$$(C_5Me_5)_2Mo_2(S_2)S_2 + Co_2(CO)_8 \longrightarrow Cp_2Mo_2Co_2S_4(CO)_2 + 6CO \tag{4}$$
$$Cp_2Mo_2(\mu\text{-}S)_2(\mu\text{-}SH)_2 + Fe_2(CO)_9 \longrightarrow Cp_2Mo_2Fe_2S_4(CO)_6 + 3CO \tag{5}$$

While only a small amount of time has been spent on this organometallic approach, $(NEt_4)_2\{Ni(SPh)_4[Mo(CO)_4]_2\}$ and $(NEt_4)_2\{Co(SPh)_4[Mo(CO)_4]_2\}$ have been synthesized and characterized by infra-red (IR) spectroscopic methods.

Approach 2. Two grams of each Chevrel phase ($HoMo_6S_8$, $SmMo_6S_8$, $AgMo_6S_8$, $InMo_6S_8$, $Cu_{3.2}Mo_6S_8$, $Fe_{1.5}Mo_6S_8$, $Ni_{1.6}Mo_6S_8$, $Co_{1.63}Mo_6S_8$) have been prepared and characterized by X-ray powder diffraction techniques. Mo_2S_3 was found as an additional phase in the $HoMo_6S_8$ and $SmMo_6S_8$ preparations. In order to ensure that pure Chevrel phase material is being produced, a second grinding and heating step will be added for the lanthanide compounds to facilitate complete reaction.

Approach 3. Using the same vapor phase reaction procedure that was given in the previous quarterly report (TPR8), $Mo(CO)_6$ and H_2S have been reacted at 300°C to produce a material with apparent high surface area. The resulting material has been shown by X-ray powder diffraction to be essentially amorphous. This is a strong indication of smaller particle size at the lower temperature, 300°C, relative to previous materials produced at 500-1100°C. A series of molybdenum materials produced from this vapor phase technique using H_2S have been sent to UCC&P for compositional, morphological and surface analyses. Preliminary results indicate that, in contrast to the surface-area dependence on furnace temperature, MoS_2 can be produced at all temperatures used in this study.

Additionally, using a similar procedure, $Mo(CO)_6$ and ammonia have been reacted to form powders amorphous to X-rays. To date, the reactions with ammonia have been performed at 200, 300, 400, and 500°C. Analogous to the H_2S studies, a relationship between furnace temperature and grain size appears to be present. The molybdenum nitrides/carbides were studied with X-ray powder diffraction and SEM. From the X-ray diffraction patterns in Figure 1, Bragg diffraction peaks can be seen growing in at higher temperatures, correlating to larger grain size. SEM micrographs indicate a higher degree of agglomeration for materials produced at higher temperatures. The broad peaks present in X-ray patterns of materials produced at 300, 400, and 500°C correlate to a cubic Mo_2N (or Mo_2C) phase. It is difficult to determine the exact phase present without compositional data.

$Co_2(CO)_8$ has been replaced with tricarbonylnitrosylcobalt(0) as the volatile cobalt source for reactions potentially producing bimetallic Mo/Co sulfides and nitrides. $Co_2(CO)_8$ is difficult to manipulate due to its thermal instability. The nitrosyl compound has been shown to exhibit adequate thermal stability. We have synthesized $Co(CO)_3(NO)$ by a reaction between NO and $Co_2(CO)_8$, but many products of decomposition were observed. Thus, a more convenient synthesis of $Co(CO)_3(NO)$ has been identified and will be used. In addition, $Fe(CO)_5$ is currently being tested for reactivity in the gas phase reactor. Preliminary experiments have shown that material produced from the vapor phase decomposition of $Fe(CO)_5$ in a He atmosphere is highly pyrophoric.

Approach 4. The "$MoNN_3$" compound, which has been described in a previous quarterly report, TPR7, has been further characterized. Preliminary single-crystal studies on the nitride precursor, "$MoNN_3$" have been performed. The actual structure appears to contain oligomers formed by eight molybdenum atoms interconnected by bridging nitride ligands. In addition to the bridging ligands, there are terminal nitride and terminal azide groups. The structure of this material appears to be comprised of 1-, 2-, 3- or 4-coordinate nitrogen atoms and 6-coordinate molybdenum atoms. The crystals decomposed over the period of data collection, resulting in a relatively poor data set. Because of this decomposition, Psi scans could not be collected, therefore a suitable absorption correction could not be applied. Current efforts are focused on growing additional crystals for further X-ray studies.

1.2.3 Transition-Metal-Oxide Catalyst Research

Research was again severely limited by the temporary unavailability of UCC&P personnel. The problem was brought about by the pending retirement of two key personnel, and the resulting reorganization and reassignment of staff. We have worked our way out of the problem by shifting most catalyst synthesis research to the UCC&P Catalysis Skill Center.

1.2.4 Reaction Engineering

During this period, we have conducted an extensive literature search on the kinetics of higher-alcohol synthesis (HAS) with the aim of finding or, if necessary, developing a comprehensive kinetic model capable of predicting the yield of each alcohol, rather than lumping all of the alcohols into one pseudo-species. This kinetic model would then be used in the reactor models we have developed so far, to provide a more-realistic evaluation of the performance of the HAS reactors.

Our efforts have led us to focus on the extensive publications of the Lehigh group, led by Professor Klier, and the Italian group, led by Professor Tronconi. We are currently evaluating the approaches and the data obtained by both these groups in order to determine the most appropriate means of adopting their results for use in our task.

During this period, we have also employed STIFF3, a stiff ordinary differential equation (ODE) solver which is totally different from the LSODE package used earlier. Using STIFF3, we have solved the packed-bed/membrane reactor model developed in the previous two quarterly reports, and have confirmed the simulation results reported there.

Reaction Engineering work at UCC&P was similarly restricted by the temporary unavailability of key personnel, aggravated by an exceptionally high workload of high-priority commercial work in the Reaction Engineering Laboratories. We believe that these problems have been resolved by the assignment of additional staff to these laboratories.

1.3 Conclusions and Recommendations

The development of the catalyst testing laboratory at WVU is proceeding.

Synthetic preparations and characterizations of molybdenum-based catalysts are ongoing for the four approaches detailed in TPR8.

The literature search for detailed kinetic models of HAS has focussed on the work of two groups of researchers. Numerical results obtained earlier have been confirmed.

1.4 Future Plans

We expect the catalyst testing laboratory at WVU to be operational before the end of the next quarter. We will start shake-down using well-characterized catalysts used previously for methanol synthesis to verify the suitability of the reactors and the analysis systems.

Synthesis of catalyst candidate compounds will continue. The single remaining chevrel-phase compound mentioned in TPR8, $SnMo_6S_8$, will be synthesized according to the procedure for Approach 2 described in that quarterly report. In addition, a Pb-containing chevrel phase compound will be analogously synthesized. Surface areas of these two species will be obtained.

The high-temperature gas-phase reaction technique of Approach 3 represents a novel synthetic approach to MoS_2. In order to determine the maximum surface area for MoS_2 prepared by this technique, additional experiments will focus on determining the minimum temperature at which MoS_2 can be formed.

Samples of MoS_2 resulting from these experiments will be evaluated for their catalytic activities. Additional vapor phase reactions involving ammonia and $Mo(CO)_6$ will be performed at temperatures ranging from 600 to 1100°C. Surface area, XPS and compositional analyses of these materials will be accomplished to determine more fully the influence of temperature on physical properties. In other future efforts, emphasis will be placed on extending this approach to the preparation of mixed metal Co-Mo and Fe-Mo sulfide and nitride materials.

Future work in Approach 4 will include the preparation of a supported metal nitride and a systematic investigation of the influence of alkali doping on the catalytic behavior of these supported and unsupported molybdenum nitrides. This is detailed in TPR8.

The search for suitable kinetic models to understand the details of HAS will continue. We expect to evaluate the approaches of the Lehigh group and the Italian group to determine the most appropriate means of using their results in our models of the various reactors described in TPR7 and TPR8.

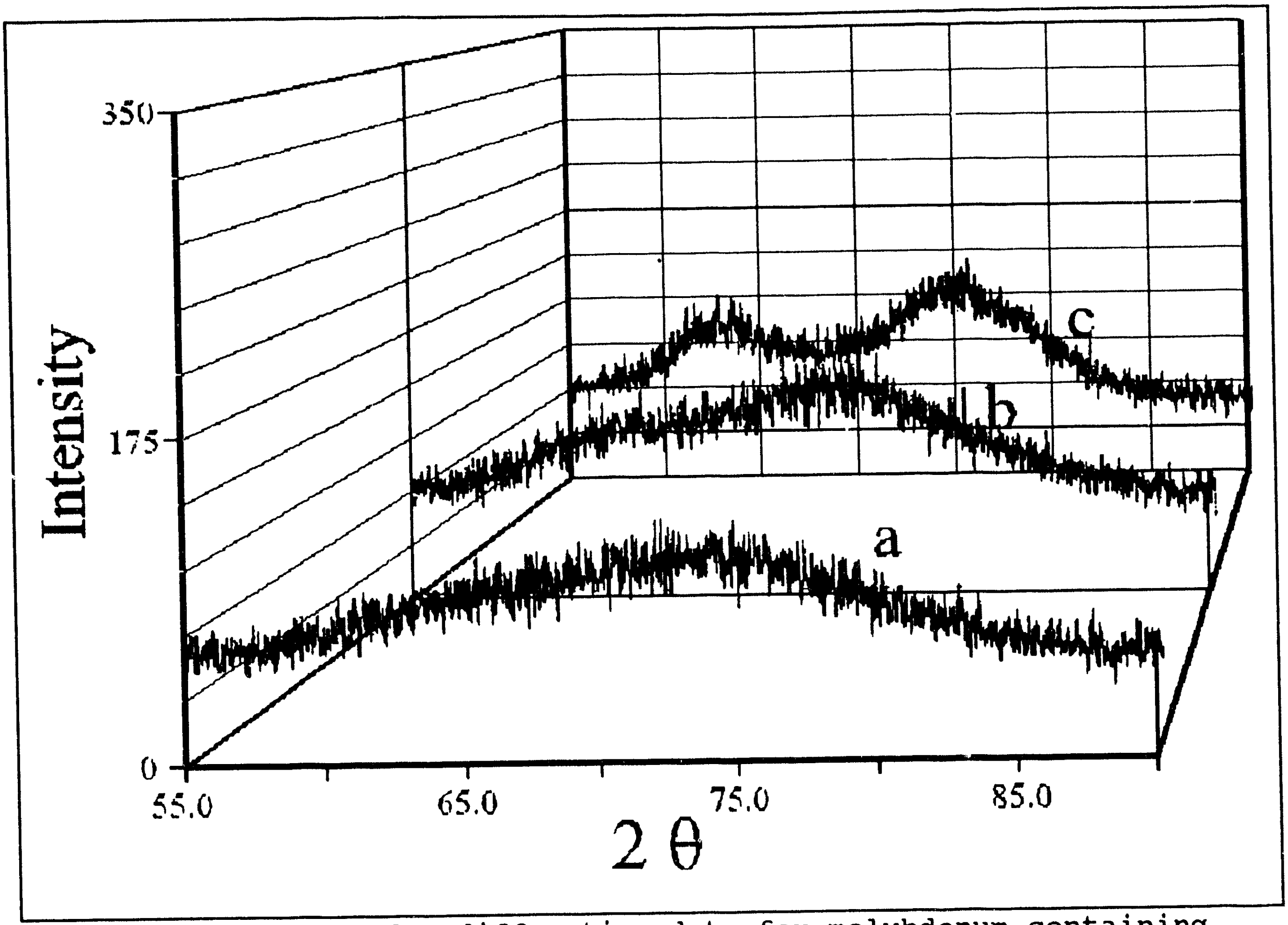

Figure 1. X-ray powder diffraction data for molybdenum containing compounds produced from vapor phase reactions between $Mo(CO)_6$ and ammonia at 300 (a), 400 (b), and 500 °C (c).

TASK 2. PROCESS SYNTHESIS AND EVALUATION

2.1 Introduction

It has been established that an energy park is a combination of facilities that utilizes one or more types of fuel with one or more types of conversion technologies to produce more than one product with the goal of reducing costs through the production of by-products, increased energy efficiency, and reduced pollution. All of these elements have been examined on an individual basis with the exception of the overall efficiency of the various processes. It is, therefore, important to focus on this final element. Once this final element of the energy park has been addressed, the basis for a more complex integrative analysis will be in place. This analysis will consider the interaction of each these elements. A model is currently being developed specifically for this purpose.

Techniques have been developed to examine process uncertainty and to optimize the alcohol production process. Process uncertainties are being examined using Monte Carlo simulations, and a methodology for this is described in this report. Simulated annealing is being used to determine the optimum separation scheme for the mixed alcohol product in order to produce blends with appropriate BRVP, octane number and oxygen content for blending with existing grades of gasoline. The methodology for this optimization is described.

In fuels testing, the work accomplished in this quarter focused on developing the software and controls for the CFR engine and the emission models that EPA has developed, the simple model and the complex model.

2.2 Accomplishments, Results and Discussion

2.2.1 Design and Energy Park

In the discussion of the energy park contained in the Third Quarter report for 1993, it was suggested that overall energy efficiencies may be used as screening mechanisms. Therefore, the overall thermal efficiencies and distribution of energy flows for the various base cases have been calculated to assess the viability of this process. These calculations were based upon the original design capacities of approximately 1500 metric tons of mixed alcohol produced per day. The total energy input and output for each of these base cases is summarized in Table 2.1. (A more detailed analysis may be found in the Appendix.) Upon examination of this information, it can be seen that the most efficient processes are those which involve the use of natural gas. Of these processes, the steam reformation of natural gas (Base Case 3) yields the best overall efficiency. Closer examination of this process however, reveals that only 36.2 percent of the total energy input actually goes to the production of alcohol. Given that the objective is to produce as much alcohol as possible, Base Case 6 may provide better results in spite of its lower overall efficiency. This may be attributed to the fact that it has the highest efficiency with respect to alcohol conversion at 56.1 percent. However, the amount of natural gas consumed by these processes imposes a series of logistical problems, if these facilities are located in remote areas not accessible to the major natural gas distribution lines.

Table 2.1

Overall Energy Efficiencies and Distributions for Base Case Designs

Base Case	1	2	3	4	5	6
Energy Input MM KJ/hr						
Coal	2959.98	8208.52	0.00	4121.25	3615.17	1825.29
Natural Gas	622.07	0.00	4701.60	0.00	0.00	1094.74
Steam	65.82	0.00	27.60	0.00	0.00	115.52
Total	3647.86	8208.52	4729.20	4121.25	3615.17	3035.56
Energy Output MM KJ/hr						
Alcohol	1712.02	1711.89	1711.89	1712.11	1701.37	1702.94
Electricity	424.80	793.44	159.48	529.56	308.16	225.36
H2	0.00	1006.96	1609.27	0.00	0.00	0.00
Light Coal Oil Mix	0.00	837.07	0.00	0.00	0.00	0.00
Total	2136.82	4349.37	3480.64	2241.67	2009.53	1928.30
Losses	1511.05	3859.15	1248.56	1879.58	1605.64	1107.26
Energy Flows						
conversion to alcohol	46.93%	20.86%	36.20%	41.54%	47.06%	56.10%
conversion to electricity	11.65%	9.67%	3.37%	12.85%	8.52%	7.42%
conversion to H2	0.00%	12.27%	34.03%	0.00%	0.00%	0.00%
conversion to coal oil	0.00%	10.20%	0.00%	0.00%	0.00%	0.00%
conversion loss	41.42%	47.01%	26.40%	45.61%	44.41%	36.48%
TOTAL EFFICIENCY	58.58%	42.79%	73.60%	54.39%	55.59%	63.52%

Base Case 6, for example, uses approximately 7.8 billion cubic feet of natural gas a year to produce approximately 500,000 metric tons of alcohol. This is equivalent to roughly 16 percent of the commercial gas consumption for the state West Virginia. If this facility's capacity is increased by a factor of eight, as proposed in previous reports, the amount of natural gas consumed by this facility would be equivalent to approximately 60 percent of the total natural gas consumption of this state. The possibility of supplementing commercial natural gas with coal bed methane was examined under the premise that it might provide some relief to the potential regional supply problems associated with the use of such large quantities of natural gas. Unfortunately, the quantity and quality of this gas proved to be insufficient for use in this capacity since it is believed that it is only possible to recover 30% to 50% of coal bed methane. This is summarized in Table 2.2.

Table 2.2
Potential of Coal Bed Methane to Supplement H_2 in Syngas

EPA estimates of methane vented globally as a result of coal mining, in billions of cubic ft		1736 to 3366
U.S. coal production as % of world coal production	18	
West Virginia coal production as % of U.S. coal production	30	
Estimated methane vented as a result of mining in WV, in billions of cubic ft		94 to 182
Methane required for Base Case 6 @ annual production of 32 MM bbl/yr higher alcohols		62.3
Methane requirement for Base Case 6 as % of estimated vented level for WV		34 to 67

Confronted with these potential problems, it appears that one of the less efficient technologies, which relies entirely on coal, may ultimately provide a feasible solution. Base Case 5 which uses a Shell gasifier in conjunction with a sour gas shift converter appears to be only slightly less efficient than its counterpart Base Case 6, which uses steam reformation of natural gas to increase the hydrogen content of the syngas. The difference between the overall efficiencies of these two base cases is approximately eight percent. This gap is relatively small and may be reduced by simply recovering a small portion of the energy losses. One potential source of recoverable energy may be the heat in the vented flue gases. This heat could be recovered and used to produce additional steam for generation of electricity. However, to determine its economic viability, the marginal cost of recovering this energy must be weighted against the marginal benefits it would provide in the form of enhanced overall efficiency.

2.2.2 Multi-Objective Model Development

The simple screening technique described above appears to be effective since it yields the same results as earlier cost analysis. However, it may not capture all of the complex interactions of the components of an energy park. Most analysis of this type have a single overriding objective. In the case described above, the objective is to maximize the overall efficiency of each processes. However, it may not be realistic to assume that a complex entity such as an energy park has a single overriding objective. In fact studies have indicated that operation of complex entities such as these may be represent more accurately through the use of multiple objectives. A multiple objective model is therefore being constructed to determine the economic feasibility of the proposed energy park in such an environment. This model will be based on Hillier and Lieberman's weighted goal programming approach which follows:

Subject to:

$$Min\ Z=\sum_{k=1}^{K}(W^{+}{}_{k}Y^{+}{}_{k}+W^{-}{}_{k}Y^{-}{}_{k}) \qquad (1)$$

$$\sum_{j=1}^{n}c_{j_k}x_j-(Y^{+}{}_{k}-Y^{-}{}_{k})=g_k,\ for\ k=1,2,\ldots,K \qquad (2)$$

and

$$Y^{+}{}_{k}\geq 0,\ Y^{-}{}_{k}\geq 0,\ x_{j},\geq 0\ (j=1,2,\ldots,n) \qquad (3)$$

where

Z = the weighted sum of the deviations of each objective function and its corresponding goal

Y_k^+ = the auxiliary variable for exceeding the goals

Y_k^- = the auxiliary variablefor under achieving the goals

W_k^+ = the penalty weight for exceeding the goals

W_k^- = the penalty weight for under achieving the goals

x_j = the activity (gasifier technology), j=1,2,3

C_{jk} = the activity's contribution to the goals

g_k = the individual goals, k=1,2

The basic idea of this model is to establish a specific numerical goal for each of the objectives, formulate an objective function for each objective, and then seek a solution that minimizes the sum of the deviations of these objective functions from their respective goals. Since some goals may be more important than others, weights may be assigned to account for theses differences. Furthermore, even for a particular goal, deviations in one direction may be more significant than deviations in the opposite direction. These differences can be taken into consideration by assigning different weights, W_k^+ and W_k^- ($k = 1,2,\ldots,K$) to the respective Y_k^+ and Y_k^- deviations, where these weights measure the relative significance of the adverse consequences that would result from these deviations.

2.2.3 Evaluation of Process Uncertainties

One of the most important concerns in a process simulation is the sensitivity of a design to the variation of parameters in the model. Related closely to this is determination of the uncertainty of the design, and the relation of this to the uncertainty of the parameters. A linear sensitivity analysis technique can determine how much the design output will change with a given change in a model parameter, but it does not provide an estimate of how likely such a variation is, nor does it address the nonlinear sensitivity. The approach proposed here provides a method which determines estimates of the design's uncertainty from simulations based upon the uncertainty of the input parameters. Also, it can determine which parameters are most significant in the design, and thus can help one make decisions concerning risk, flexibility of the plant, and when more data may be useful in model building.

This Monte Carlo procedure involves running a process model numerous times while changing the inputs to the model every time. The Monte Carlo method varies all parameters randomly and simultaneously, so cross effects can be determined. The values of each of the input parameters are chosen based on the assigned probability distribution. The necessary number of runs of the model depends on the constraints of time, accuracy, and others. The result is a set of sample values for each of the outputs that can be treated statistically as if they were an observed set of data. To run a Monte Carlo simulation, a method must be chosen to determine the input samples. For every input parameter, a set of inputs must be chosen to sample the distribution accurately. We have experience in the application of Monte Carlo simulation to process design sensitivity analysis (2-4).

There are two important applications of these techniques. First, decisions concerning the type and amount of data needed to improve the model can be made. Once the correlation coefficients are determined, it may be ascertained which parameters have the most influence on the uncertainty of the design. The next step is to estimate the effect of more data by changing the probability distribution of the input parameters that have been selected in the research. These new distributions are then used in a repetition of the analysis previously used. The results of the new calculations are compared with the first to assess the effect of the reduction of the deviation resulting from more data on the parameter. If the addition of more data causes a significant reduction, then this is recommended for further study. If new data have little or no effect on the uncertainty of design, then it is recommended that there is no need to gather more data. Second, the uncertainty of the input parameters can be quantified so that the design of equipment in the process allows for it. The design of the facility can permit a range of possible outcomes instead of using standard safety factors that may be too large or too small to meet the needs of the process.

With use of the Monte Carlo technique, several output parameters may be determined and studied. We will be able to assign a cumulative frequency to the possible values of the parameter, and rank the variables so as to determine their influence on the outcome parameters. Output variables which reflect the efficiency and cost effectiveness of the facility include its payback period, cost of product, and equivalent annual operating cost. The input variables which affect these parameters are numerous, and many can be varied within their predicted deviation. An important constraint on the parameters is that they be independent of each other, so that the uncertainties of one are not added on to another. These include the costs of coal, electricity, and natural gas; the operating temperature and pressure of the units in the process; the possible distribution of chemicals leaving the reactor; and the installed costs of the units. An important note is that the number of input variables does not affect the number of simulation runs required for a given level of confidence. Another group of variables to be considered is the parameters of the thermodynamic model used to determine the operating conditions of the units and streams in the facility. These include critical constants, acentric factors and interaction parameters for the chemicals employed in the process. Input parameters will be tested for fluctuations and uncertainties, not for optimum value. For instance, if the operating temperature of the gasifier is chosen as an input parameter, it will be tested for amount of deviation possible from the value used in the simulation. Our studies will indicate how much this fluctuation effects the process, not what the best operating condition will be.

One parameter that takes all this into account is the Energy Efficiency of the facility. This can be calculated by determining the difference between the amount of power (e.g., electricity, steam) entering and leaving the plant, and the total heating value of the materials entering and leaving the plant. The efficiency is then found by summing the difference in power entering and leaving and the differences in the sum higher heating values of pertinent chemicals entering and leaving the plant. As this difference decreases, the facility increases in its efficiency of energy use, thus reducing the cost of production of the end products. Another such parameter is the Payback Period of the facility. This calculation is determined by dividing the cost to build the facility by the annual margin of cash flow. The margin is the difference between the revenue from the produced chemicals and the costs of raw materials and operating expenses. This parameter takes into account both the initial cost of building the plant and the margin between operating costs and sales revenue. Decreases in equipment sizes and utilities, or increases in production will decrease the payback period, thus improving the profitability of the facility.

2.2.4 Optimization

The syngas is primarily converted into alcohols, water, esters in the reactor. Methanol and ethanol comprise the bulk of the alcohols. Before the alcohols can be used as gasoline additives they must be separated (at least partially) so that they can be mixed into appropriate blends. A network of distillation columns is used to perform the task of creating streams rich in certain alcohols so that a blend approved by the EPA can be formulated by mixing the alcohol stream with straight run gasoline and n-butane.

The network of distillation columns perform two distinct key component separations, namely, methanol/ethanol and ethanol/propanol. These separations create streams rich in methanol or ethanol or higher alcohols along with a number of side streams which might be rich in a combination of alcohols. The cost of separation is a function of pressure at the top and bottom of a column, the temperature of the feed, the degree of separation of the light and heavy key, the relative composition of the various components in the feed stream, the volumetric flow of the feed stream, the number of stages and the feed stage location. The cost of each column is obtained by generating cost for a number of test cases using the ASPEN costing model and regressing the cost data over the variables. The regressed equations can provide the cost of operating a column within 10% of the cost obtained from ASPEN.

The properties (BRVP, octane number, and amount of oxygen) of the stream exiting the network of distillation column is dependent on the amount of each individual alcohol in the particular stream. However, the amount of individual alcohol in a particular stream is dependent upon the operating conditions of the various columns. Thus, the operating conditions for the columns have a direct impact on the properties of the alcohol streams leaving the columns. The various alcohols have to be blended with straight run gasoline and n-butane in an appropriate manner to satisfy the BRVP, octane number and the amount of oxygen requirements of the blended product. Simulated annealing is used as the optimization technique for obtaining the various operating conditions while the blending problem is formulated as a linear programming problem and is solved using IMSL subroutines. The problem has been formulated so that the linear programming problem of blending is in the inner loop and is run each time the simulated annealing changes the random variables in the outer loop. The total profitability is the amount of revenue generated by selling the blended product after accounting for the cost of production of alcohol (installed and operating cost of reactor and distillation columns).

At present, the linear problem for the blending of the alcohols is being formulated. When incorporated with the simulated annealing program (already coded), this will provide the desired results.

2.2.5 Fuels Testing

2.2.5.1Waukesha Engine Data Acquisition System Summary

During the past quarter, work has been done to update the instrumentation setup on the Waukesha Co-operative Fuels Research Engine (CFR) . This instrumentation is being designed to allow for testing of various alcohol fuels and blends of alcohols and gasoline. The instrumentation, shown in Figure 2.1, includes the following:

I. Temperature measurements - performed with either T or K type thermocouples and signal conditioning cards.

A. Water Coolant Temperature (T Thermocouple)
B. Oil Temperature (T Thermocouple)
C. Intake Manifold Temperature (T Thermocouple)
D. Exhaust Manifold Temperature (K Thermocouple)
E. Ambient Air Temperature (T Thermocouple)

II. Pressure Measurements

A. Oil Pressure (need to buy a transducer)
B. Intake Manifold Pressure (Omega PX-AV30 0-30 psia transducer)
C. Exhaust Manifold Pressure (need to buy a transducer)
D. In Cylinder Pressure (PCB transducer)

III. Intake Air Flow rate Measurement

This is done via Sponsler SP3/4-CB-PHL-B-4RFX flowmeter with an SP718-V-12_5 sending unit. This setup is capable of reading 0.04-3 CFM.

IV. Crank Angle

The crank angle will be read with PEI Motion Systems angle encoder which can read to the nearest 1/2 degree.

The objective now is to complete the installation of various transducers and to complete the computer program that will eventually read all the data and store it or display it. The program is being written in the Microsoft Professional BASIC Development System. The program will be user-friendly and goof-proofed. Data will be displayed via dial gages and bar gages which will appear on the screen, and the program will contain a calibration routine for calibrating any of the above mentioned transducers. In addition, the program will be capable of displaying traces of in-cylinder pressure vs. crank angle, and it will be able to save these traces in a data file which can be imported into graphing or spreadsheet packages. With these pressure traces, it should be possible to determine the amount of "knocking" that would be occurring in the cylinder with different fuel types.

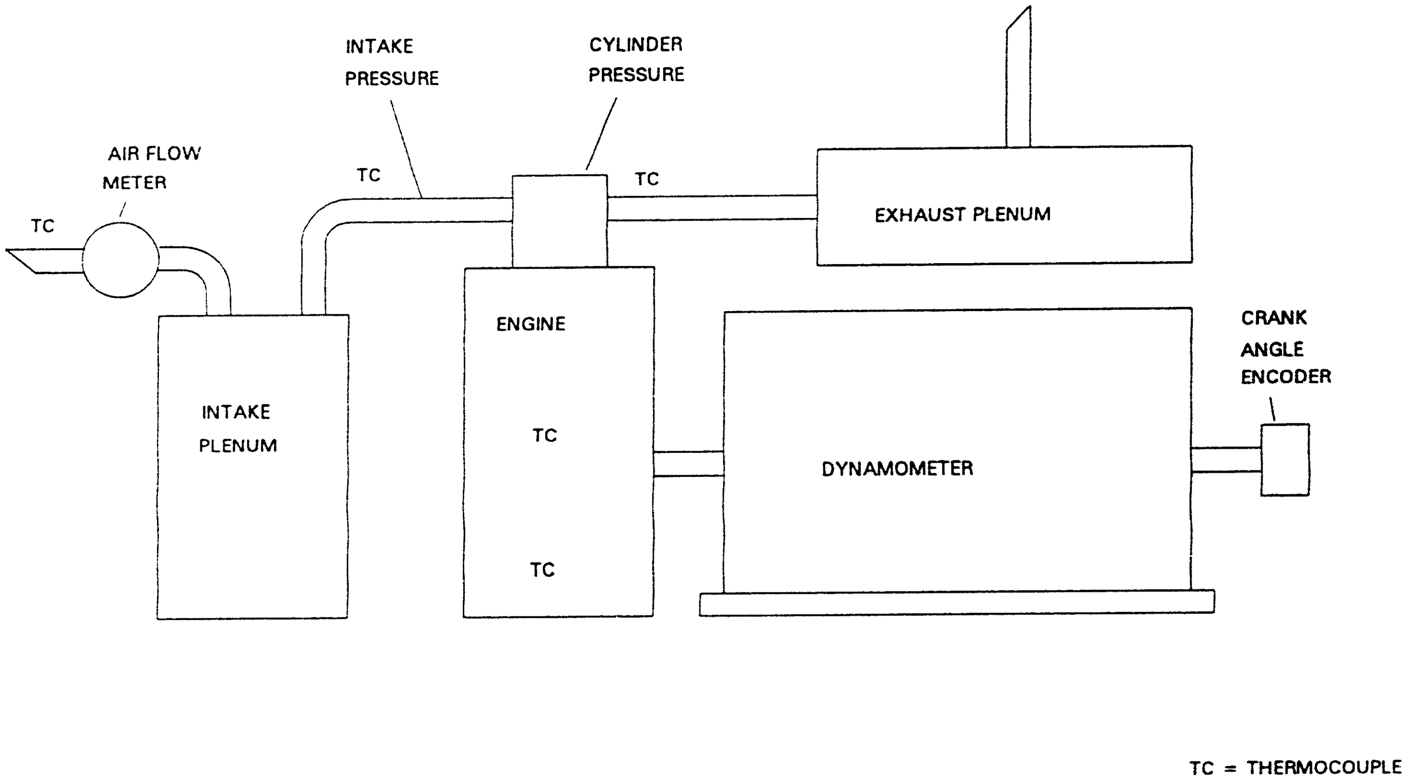

Figure 2.1: Waukesha Engine Data Acquisition System

2.2.5.2Emissions Models Developed EPA

EPA has developed a non-exhaust model, called the Simple Model, which is valid through Dec. 31, 1993. This model predicts the evaporative, refueling and running losses from vehicles operating on various fuels. The model does not consider the exhaust emissions. It is based on the RVP, the oxygen content (percentage weight oxygen in MTBE, ETBE, TAME, ETAE, EtOH), the aromatics, and benzene for the Class C and Class B fuels. The RVP and the oxygen content are used for predicting the volatile organic compounds. Aromatics and benzene are used for predicting the toxics emissions. The total toxics (expressed in mg/mile) include the benzene, butadiene, formaldehyde and acetaldehyde emissions.

The model applicable from Jan. 1, 1993 will be the complex model for VOC, toxics and oxides of nitrogen (NO_x). The model requires eight parameters, such as weight percentage oxygen, sulfur (ppm), RVP (psi), two points on the distillation curve - E200 and E300 (in %), aromatics (vol %), olefins (%) and benzene (%) in the fuel. The predicted emissions are in mg/mile for the total (exhaust and evaporative) VOC; and the total toxics (exhaust and evaporative benzene; acetaldehyde, butadiene and acetaldehyde, POM); and NO_x. The emissions from the target fuel can be compared against the baseline fuel that has been provided by the model.

The model now, provides the alcohol fuels group with guidelines and targets that need to be met and will assist in the final composition of the proposed alcohol and gasoline blend.

2.3 Conclusions and Recommendations

The use of overall efficiencies as a screening tool may not fully explain the complexities of an energy park. However, it does provide an effective means for selecting alternative technologies. This is exemplified by the fact that the same conclusions are derived by this method and the cost analysis conducted earlier. Both methods emphasize the fact that the use of natural gas in the production process enhances the economics of the process. These results should not be astonishing since efficiency and cost are interrelated. However, this investigation may have revealed some potential recoverable energy in the flue gases loses which could possibly reduce operating cost and enhance the economics.

The possibility of recovering these energy losses needs to be investigated further to determine their economic feasibility. To do this, cost data must be obtained for this heat recovery process. The amount of additional electricity generated from the steam supplied from this process must also be determined. Once this information is obtained, the cost may be weighed against the benefits to determine the economic viability of this process. However, the potential to recover this lost energy exists for all the base cases; therefore, the coal cases are not expected to benefit disproportionately. Production techniques using natural gas will inevitably remain more economical, thus driving the location of this facility to a region containing ample supplies of both coal and natural gas.

Additional personnel, with expertise in instrumentation, controls and software were hired in the fuels testing group, and have been working very effectively in installing the data acquisition system and data reduction program on the engine. Individual modules of the program have been successfully tested and this usually forms the bulk of an experimental study. Recent experiences with running alcohol blends in the engine have provided the necessary expertise in gathering emissions and performance data from the engine, and have provided an estimate of the time it requires.

The complex model for VOC, toxics and the NO_x will be used as a guideline for deciding the final composition of the proposed blend and the results will be checked against the experimental data.

2.4 Future Plans

The focus for the next several months is to continue with the energy park analysis, the optimization, and the uncertainty analysis. The energy park analysis will focus on the multiple objective analysis in order to evaluate the economic feasibility of the energy park concept. Furthermore, work at Union Carbide will focus on use of the Advent® pinch technology software to determine energy efficient process configurations. Optimization studies will continue to focus on the alcohol synthesis and separation portion of the process. However, a methodology for using simulated annealing to optimize the syngas generation portion of the process will also be investigated. Finally, the uncertainty analysis will focus on determining the probability distributions for input parameters. For input parameters such as raw material costs, the history of these costs will be used. For input parameters such as equipment operating conditions, engineering judgment will be required.

For the past quarter, the emphasis in fuels testing was devoted to updating the CFR engine and developing the software. The next quarter will be devoted to extensive engine tests on various blends for performance and emissions evaluations.

2.5 Appendix 1 for Task 2

There are six tables in the Appendix. These present a more detailed energy analysis of the base cases. Details of these base cases may be found in previous quarterly reports. For reference, the base cases were as follows:

Base Case 1	Texaco Gasifier and Natural Gas
Base Case 2	Lurgi Gasifier
Base Case 3	Natural Gas Only
Base Case 4	Texaco Gasifier and Sour Gas Shift Converter
Base Case 5	Shell Gasifier and Sour Gas Shift Converter
Base Case 6	Shell Gasifier and Natural Gas

Table A2.1: Base Case 1 Energy Analysis

1 kJ = 0.9486 Btu
1 kg = 2.20462 lb

STEAM

Steam Used

Steam Type	Rectisol Plant (kg/hr)	Cryogenic Oxygen Plant (kg/hr)	Syn. Gas Heat Recovery Plant (kg/hr)	Stream 76 Steam Turbine (kg/hr)*	Stream 15 Syn. Gas from N.G. (kg/hr)
29psig (200kPa)	0	0	0	0	1700
50psig (345kPa)	21000	0	0	0	0
100psig (690kPa)	2900	0	0	0	0
250psig (1724kPa)	0	5500	0	0	0
700psig (4826kPa)	0	0	0	0	0
900psig (6205kPa)	0	17400	8900	0	0
1500psig (10446kPa)	0	0	0	19200	0

* Steam leaving the turbine is at 1 psig and 82C

Steam Produced

Steam Type	Claus Plant (kg/hr)	Stream 68 Syn. Gas Heat Recovery Plant (kg/hr)	Stream 74 Syn. Gas Combustion (kg/hr)
29psig (200kPa)	0	0	0
50psig (345kPa)	2800	0	0
100psig (690kPa)	0	0	0
250psig (1724kPa)	0	0	0
700psig (4826kPa)	3900	0	0
900psig (6205kPa)	0	0	0
1500psig (10446kPa)	0	12700	6500

Steam Totals

Steam Type	Total Steam Used (kg/hr)	Total Steam Produced (kg/hr)	Heat Content (kJ/kg)	Steam Used (kJ/hr)	Steam Produced (kJ/hr)
29psig (200kPa)	1700	0	2208	3753600	0
50psig (345kPa)	21000	2800	2166.2	45490200	6065360
100psig (690kPa)	2900	0	2071.7	6007930	0
250psig (1724kPa)	5500	0	1920	10560000	0
700psig (4826kPa)	0	3900	1654	0	6450600
900psig (6205kPa)	26300	0	1571	41317300	0
1500psig (10446kPa)	19200	19200	1320	25344000	25344000

Base Case 1 cont.

ELECTRICITY

Plant	Electricity Used (MW)	Electricity Produced (MW)
Coal Preparation Plant	1.6	0
Cryogenic Oxygen Plant	1.3	0
Rectisol Plant	1.9	0
Texaco Gasifier	0.5	0
Syn. Gas Heat Recovery	0.7	0
Claus Plant	0.1	0
Gas Turbine	0	2
Steam Turbine	0	116
Compressor 1	25.3	0
Compressor 2	7.9	0
Compressor 3	12.3	
Compressor 4	6	0
Compressor 5	1.6	0
Total	59.2	118

Heating Values
COAL and ALCOHOLS

1 kJ/kg = 0.43028 Btu/lb
1 kJ/kmol = 0.43028 Btu/lbmol

Inlet	Heating Value			
	(kJ/kg)	(kJ/kmol)	(Btu/lb)	(Btu/lbmol)
Coal	-29054	-331506.14	-12501.30	-142639.88
Natural Gas	-55486	-890161.9	-23874.42	-383017.29

Outlet	Heating Value			
	(kJ/kg)	(kJ/kmol)	(Btu/lb)	(Btu/lbmol)
Alcohols	-27430	-1168792.3	-11802.53	-502905.89

Table A2.2: Base Case 2 Energy Analysis

1 kJ = 0.9486 Btu
1 kg = 2.20462 lb

STEAM

Steam Used

Steam Type	Rectisol Plant (kg/hr)	Cryogenic Oxygen Plant (kg/hr)	Stream 76 Steam Turbine (kg/hr)*
29psig (200kPa)	0	0	0
50psig (345kPa)	83000	0	0
100psig (690kPa)	11300	0	0
250psig (1724kPa)	0	9600	0
700psig (4826kPa)	0	0	0
900psig (6205kPa)	0	30200	0
1500psig (10446kPa)	0	0	33000

* Steam leaving the turbine is at 1 psig and 82C

Steam Produced

Steam Type	Claus Plant (kg/hr)	Stream 74 Syn. Gas Combustion (kg/hr)
29psig (200kPa)	0	0
50psig (345kPa)	7500	0
100psig (690kPa)	0	0
250psig (1724kPa)	0	0
700psig (4826kPa)	10500	0
900psig (6205kPa)	0	0
1500psig (10446kPa)	0	33000

Steam Totals

Steam Type	Total Steam Used (kg/hr)	Total Steam Produced (kg/hr)	Heat Content (kJ/kg)	Steam Used (kJ/hr)	Steam Produced (kJ/hr)
29psig (200kPa)	0	0	2208	0	0
50psig (345kPa)	83000	7500	2166.2	179794600	16246500
100psig (690kPa)	11300	0	2071.7	23410210	0
250psig (1724kPa)	9600	0	1920	18432000	0
700psig (4826kPa)	0	10500	1654	0	17367000
900psig (6205kPa)	30200	0	1571	47444200	0
1500psig (10446kPa)	33000	33000	1320	43560000	43560000

Base Case 2 cont.

ELECTRICITY

Plant	Electricity Used (MW)	Electricity Produced (MW)
Coal Preparation Plant	4.5	0
Cryogenic Oxygen Plant	2.3	0
Rectisol Plant	7.3	0
Claus Plant	0.3	0
Gas Turbine	0	11.6
Steam Turbine	0	208.8
Compressor 1	44	0
Compressor 2	13.7	0
Compressor 4	7	0
Compressor 5	1.6	0
Total	80.7	220.4

Heating Values
COAL and ALCOHOLS

1 kJ/kg = 0.43028 Btu/lb
1 kJ/kmol = 0.43028 Btu/lbmol

Inlet	Heating Value			
	(kJ/kg)	(kJ/kmol)	(Btu/lb)	(Btu/lbmol)
Coal	-29054	-331506.14	-12501.30	-142639.88

Outlet	Heating Value			
	(kJ/kg)	(kJ/kmol)	(Btu/lb)	(Btu/lbmol)
Alcohols	-27430	-1168792.3	-11802.53	-502905.89

Table A2.3: Base Case 3 Energy Analysis

1 kJ = 0.9486 Btu
1 kg = 2.20462 lb

STEAM

Steam Used		
Steam Type	Stream 76 Steam Turbine (kg/hr)*	Stream 15 Syn. Gas from N.G. (kg/hr)
29psig (200kPa)	0	12500
50psig (345kPa)	0	0
100psig (690kPa)	0	0
250psig (1724kPa)	0	0
700psig (4826kPa)	0	0
900psig (6205kPa)	0	0
1500psig (10446kPa)	6200	0

* Steam leaving the turbine is at 1 psig and 82C

Steam Produced	
Steam Type	Stream 74 Syn. Gas Combustion (kg/hr)
29psig (200kPa)	0
50psig (345kPa)	0
100psig (690kPa)	0
250psig (1724kPa)	0
700psig (4826kPa)	0
900psig (6205kPa)	0
1500psig (10446kPa)	6200

Steam Totals					
Steam Type	Total Steam Used (kg/hr)	Total Steam Produced (kg/hr)	Heat Content (kJ/kg)	Steam Used (kJ/hr)	Steam Produced (kJ/hr)
29psig (200kPa)	12500	0	2208	27600000	0
50psig (345kPa)	0	0	2166.2	0	0
100psig (690kPa)	0	0	2071.7	0	0
250psig (1724kPa)	0	0	1920	0	0
700psig (4826kPa)	0	0	1654	0	0
900psig (6205kPa)	0	0	1571	0	0
1500psig (10446kPa)	6200	6200	1320	8184000	8184000

Base Case 3 cont.

ELECTRICITY

Plant	Electricity Used (MW)	Electricity Produced (MW)
Rectisol Plant	0.8	0
Gas Turbine	0	1.9
Steam Turbine	0	42.4
Compressor 4	5.4	0
Compressor 5	1.7	0
Total	**7.9**	**44.3**

Heating Values
COAL and ALCOHOLS

1 kJ/kg = 0.43028 Btu/lb
1 kJ/kmol = 0.43028 Btu/lbmol

Inlet	Heating Value			
	(kJ/kg)	(kJ/kmol)	(Btu/lb)	(Btu/lbmol)
Natural Gas	-55486	-890161.9	-23874.42	-383017.29

Outlet	Heating Value			
	(kJ/kg)	(kJ/kmol)	(Btu/lb)	(Btu/lbmol)
Alcohols	-27430	-1168792.3	-11802.53	-502905.89

Table A2.4: Base Case 4 Energy Analysis

1 kJ = 0.9486 Btu
1 kg = 2.20462 lb

STEAM

Steam Used

Steam Type	Rectisol Plant (kg/hr)	Cryogenic Oxygen Plant (kg/hr)	Syn. Gas Heat Recovery Plant (kg/hr)	Stream 76 Steam Turbine (kg/hr)*
50psig (345kPa)	40300	0	0	0
100psig (690kPa)	20300	0	0	0
250psig (1724kPa)	0	7700	0	0
700psig (4826kPa)	0	0	5600	0
900psig (6205kPa)	0	24200	12400	0
1500psig (10446kPa)	0	0	0	24200

* Steam leaving the turbine is at 1 psig and 82C

Steam Produced

Steam Type	Claus Plant (kg/hr)	Stream 68 Syn. Gas Heat Recovery Plant (kg/hr)	Stream 74 Syn. Gas Combustion (kg/hr)
50psig (345kPa)	3900	0	0
100psig (690kPa)	0	0	0
250psig (1724kPa)	0	0	0
700psig (4826kPa)	5500	0	0
900psig (6205kPa)	0	0	0
1500psig (10446kPa)	0	17700	6500

Steam Totals

Steam Type	Total Steam Used (kg/hr)	Total Steam Produced (kg/hr)	Heat Content (kJ/kg)	Steam Used (kJ/hr)	Steam Produced (kJ/hr)
50psig (345kPa)	40300	3900	2166.2	87297860	8448180
100psig (690kPa)	20300	0	2071.7	42055510	0
250psig (1724kPa)	7700	0	1920	14784000	0
700psig (4826kPa)	5600	5500	1654	9262400	9097000
900psig (6205kPa)	36600	0	1571	57498600	0
1500psig (10446kPa)	24200	24200	1320	31944000	31944000

Base Case 4 cont.

ELECTRICITY

Plant	Electricity Used (MW)	Electricity Produced (MW)
Coal Preparation Plant	2.3	0
Cryogenic Oxygen Plant	1.8	0
Rectisol Plant	3.8	0
Texaco Gasifier	0.7	0
Syn. Gas Heat Recovery	0.9	0
Claus Plant	0.2	0
Gas Turbine	0	2.1
Steam Turbine	0	145
Compressor 1	35.2	0
Compressor 2	11	0
Compressor 4	5.8	0
Compressor 5	1.6	0
Total	**63.3**	**147.1**

Heating Values
COAL and ALCOHOLS

1 kJ/kg = 0.43028 Btu/lb
1 kJ/kmol = 0.43028 Btu/lbmol

Inlet	Heating Value			
	(kJ/kg)	(kJ/kmol)	(Btu/lb)	(Btu/lbmol)
Coal	-29054	-331506.14	-12501.30	-142639.88

Outlet	Heating Value			
	(kJ/kg)	(kJ/kmol)	(Btu/lb)	(Btu/lbmol)
Alcohols	-27430	-1168792.3	-11802.53	-502905.89

Table A2.5: Base Case 5 Energy Analysis

1 kJ = 0.9486 Btu
1 kg = 2.20462 lb

STEAM

Steam Used

Steam Type	Rectisol Plant (kg/hr)	Cryogenic Oxygen Plant (kg/hr)	Syn. Gas Heat Recovery Plant (kg/hr)	Stream 76 Steam Turbine (kg/hr)*
50psig (345kPa)	39500	0	0	0
100psig (690kPa)	19900	0	0	0
250psig (1724kPa)	0	6800	0	0
700psig (4826kPa)	0	0	3700	0
900psig (6205kPa)	0	21600	8200	0
1500psig (10446kPa)	0	0	0	13800

* Steam leaving the turbine is at 1 psig and 82C

Steam Produced

Steam Type	Claus Plant (kg/hr)	Stream 68 Syn. Gas Heat Recovery Plant (kg/hr)	Stream 74 Syn. Gas Combustion (kg/hr)
50psig (345kPa)	4400	0	0
100psig (690kPa)	0	0	0
250psig (1724kPa)	0	0	0
700psig (4826kPa)	6100	0	0
900psig (6205kPa)	0	0	0
1500psig (10446kPa)	0	7700	6100

Steam Totals

Steam Type	Total Steam Used (kg/hr)	Total Steam Produced (kg/hr)	Heat Content (kJ/kg)	Steam Used (kJ/hr)	Steam Produced (kJ/hr)
50psig (345kPa)	39500	4400	2166.2	85564900	9531280
100psig (690kPa)	19900	0	2071.7	41226830	0
250psig (1724kPa)	6800	0	1920	13056000	0
700psig (4826kPa)	3700	6100	1654	6119800	10089400
900psig (6205kPa)	29800	0	1571	46815800	0
1500psig (10446kPa)	13800	13800	1320	18216000	18216000

Base Case 5 cont.

ELECTRICITY

Plant	Electricity Used (MW)	Electricity Produced (MW)
Coal Preparation Plant	2	0
Cryogenic Oxygen Plant	1.6	0
Rectisol Plant	3.7	0
Syn. Gas Heat Recovery	0.6	0
Claus Plant	0.2	0
Gas Turbine	0	1.9
Steam Turbine	0	83.7
Compressor 1	31.4	0
Compressor 2	6.9	0
Compressor 4	15	0
Compressor 5	1.6	0
Total	**63**	**85.6**

Heating Values COAL and ALCOHOLS

1 kJ/kg = 0.43028 Btu/lb
1 kJ/kmol = 0.43028 Btu/lbmol

Inlet	Heating Value			
	(kJ/kg)	(kJ/kmol)	(Btu/lb)	(Btu/lbmol)
Coal	-29054	-331506.14	-12501.30	-142639.88

Outlet	Heating Value			
	(kJ/kg)	(kJ/kmol)	(Btu/lb)	(Btu/lbmol)
Alcohols	-27430	-1168792.3	-11802.53	-502905.89

Table A2.6: Base Case 6 Energy Analysis

1 kJ = 0.9486 Btu
1 kg = 2.20462 lb

STEAM

Steam Used

Steam Type	Rectisol Plant (kg/hr)	Cryogenic Oxygen Plant (kg/hr)	Syn. Gas Heat Recovery Plant (kg/hr)	Stream 76 Steam Turbine (kg/hr)*	Stream 15 Syn. Gas from N.G. (kg/hr)
29psig (200kPa)	0	0	0	0	1200
50psig (345kPa)	5900	0	0	0	0
100psig (690kPa)	800	0	0	0	0
250psig (1724kPa)	0	3500	0	0	0
700psig (4826kPa)	0	0	0	0	0
900psig (6205kPa)	0	10900	4100	0	0
1500psig (10446kPa)	0	0	0	10000	0

* Steam leaving the turbine is at 1 psig and 82C

Steam Produced

Steam Type	Claus Plant (kg/hr)	Stream 68 Syn. Gas Heat Recovery Plant (kg/hr)	Stream 74 Syn. Gas Combustion (kg/hr)
29psig (200kPa)	0	0	0
50psig (345kPa)	2200	0	0
100psig (690kPa)	0	0	0
250psig (1724kPa)	0	0	0
700psig (4826kPa)	3100	0	0
900psig (6205kPa)	0	0	0
1500psig (10446kPa)	0	3900	6100

Steam Totals

Steam Type	Total Steam Used (kg/hr)	Total Steam Produced (kg/hr)	Heat Content (kJ/kg)	Steam Used (kJ/hr)	Steam Produced (kJ/hr)
29psig (200kPa)	1200	0	2208	2649600	0
50psig (345kPa)	5900	2200	2166.2	12780580	4765640
100psig (690kPa)	800	0	2071.7	1657360	0
250psig (1724kPa)	3500	0	1920	6720000	0
700psig (4826kPa)	0	3100	1654	0	5127400
900psig (6205kPa)	15000	0	1571	23565000	0
1500psig (10446kPa)	10000	10000	1320	13200000	13200000

Base Case 6 cont.

ELECTRICITY

Plant	Electricity Used (MW)	Electricity Produced (MW)
Coal Preparation Plant	1	0
Cryogenic Oxygen Plant	0.8	0
Rectisol Plant	0.5	0
Syn. Gas Heat Recovery	0.3	0
Claus Plant	0.1	0
Gas Turbine	0	1.9
Steam Turbine	0	60.7
Compressor 1	15.9	0
Compressor 2	3.5	0
Compressor 3	14.8	
Compressor 4	6.6	0
Compressor 5	1.6	0
Total	45.1	62.6

Heating Values
COAL and ALCOHOLS

1 kJ/kg = 0.43028 Btu/lb
1 kJ/kmol = 0.43028 Btu/lbmol

Inlet	Heating Value			
	(kJ/kg)	(kJ/kmol)	(Btu/lb)	(Btu/lbmol)
Coal	-29054	-331506.14	-12501.30	-142639.88
Natural Gas	-55486	-890161.9	-23874.42	-383017.29

Outlet	Heating Value			
	(kJ/kg)	(kJ/kmol)	(Btu/lb)	(Btu/lbmol)
Alcohols	-27430	-1168792.3	-11802.53	-502905.89

2.6 References for Task 2

1. Hillier, F. and G. Leiberman, *Introduction to Operations Research (3rd ed)*, Holden-Day, San Francisco, 1980.

2. Reed, M. E., *Probabilistic Analysis of the Effect of Error in Thermodynamic Parameters on the Computer Simulated Design and Cost Estimation of Distillation Columns*, Thesis submitted to Graduate School of West Virginia University, 1992.

3. Reed, M. E., and W. B. Whiting, "Sensitivity and Uncertainty of Process Designs to Thermodynamic Model Parameters: A Monte Carlo Approach," *Chem. Engr. Commun.*, to be published (1993).

4. Whiting, W. B., T.-M. Tong, and M. E. Reed, "Effect of Uncertainties in Thermodynamic Data and Model Parameters of Calculated Process Performance," *Ind. Eng. Chem. Res.*, **32**, 1367-1371, (1993).