QUARTERLY TECHNICAL PROGRESS REPORT
NUMBER 7

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

CONTRACT NO. DE-AC22-91PC91034

REPORTING PERIOD:

April 1, 1993 to June 30, 1993

SUBMITTED TO:

Document Control Center
U.S. Department of Energy
Pittsburgh Energy Technology Center
P.O. Box 10940, MS 921-118
Pittsburgh, PA 15236-0940

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July, 1993

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Executive Summary

In Task 1, catalyst materials preparation is proceeding actively at WVU and UCC&P. Molybdenum based materials are being prepared at WVU in sulfide, nitride and oxide forms. A standard catalyst for evaluation of reaction units has been prepared at UCC&P, following the recipe described in U.S. Patent 4,943,551.

Reaction unit construction has begun at WVU and is expected to be completed by September, 1993. Reaction studies at UCC&P were delayed due to problems with online analytical equipment. These problems have been resolved.

Alcohol synthesis reaction modeling has proceeded well. Prior applications to packed bed and stirred-tank reactors have been extended to a membrane reactor model. Literature data was used to test this program.

In Task 2, an analysis of the current base cases has been undertaken to determine if the economic status of the proposed alcohol fuels may benefit from economies of scale. This analysis was based on a literature review which suggested that plants of capacities substantially below 5000 metric tons/day are unlikely to be competitive for the bulk production of alcohols for fuel consumption or chemicals manufacture. The preliminary results of this scale up procedure would indicate that the capacity of the current base cases be increased by a factor of eight. This would yield annual production of 4.1 million metric tons and essentially reduce the plant gate cost by approximately 41 percent in both cases. A facility of this size would be the equivalent of a medium sized oil refinery and would be capable of sustaining local market demands for fuel oxygenates. The actual competitiveness of this product with current oxygenates such as MTBE remains to be determined.

The alcohol synthesis loop is being used to evaluate optimization procedures which will eventually be used to optimize the entire process. A more detailed design of the synthesis reactor is required, and a preliminary design of this reactor has been completed.

A preliminary environmental analysis of the sulfur removal portion of Base Case 1 has been completed, accounting for both fugitive emissions and stack emissions. It indicates that the threshold limits for hydrogen sulfide and ozone are exceeded. This will require BACT (Best Available Control Technology), which would add yet undetermined costs to construction and operation of a coal to syngas to higher alcohols plant.

Small concentrations of esters formed during alcohol synthesis will contribute little to the corrosion of fuel storage and combustion systems; hence, their separation may not be necessary. Chloride ion should be avoided, even in small quantities, since severe corrosion is found at 10 ppm. Based upon information in the literature, gasoline-alcohol blends should contain less than 3.7 wt % oxygen. The "substantially similar" clause imposed by the EPA will have to be met before fuels produced by this process could be used on a commercial basis.

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 is focused on molybdenum based catalysts. Parallel research being done at Union Carbide Chemicals and Plastics is focused on transition metal oxide catalysts.

1.2 Accomplishments, Results and Discussion

1.2.1 Laboratory Setup

Catalyst testing facilities at WVU are currently under construction. Details on the unit designs were provided in Quarterly Technical Progress Report 5, January 1993.

At UCC&P there are four reaction systems for testing catalysts and obtaining kinetic data.

1) Tubular microreactors for small scale gas-solid reactions.

2) A Berty autoclave reactor for gas-solid kinetic studies.

3) A slurry autoclave reactor for three phase reactions.

4) An *in situ* FTIR reaction system for online analysis of products and intermediates.

There have been problems with the gas chromatography analytical equipment in this lab which delayed catalyst testing. These problems seem to have been resolved with the help of the UCC gas chromatography specialists.

1.2.2 Molybdenum Based Catalyst Research

Molybdenum catalyst preparations are being investigated using four approaches:

1) Synthesis and thermal decomposition of heterobimetallic

inorganic and organometallic sulfide compounds.

2) Synthesis of supported and unsupported Chevrel phase compounds ($M'Mo_6S_8$) through the use of water soluble and refractory precursors.

3) Elevated temperature vapor phase synthesis of mixed metal sulfides and/or nitrides by the reaction of volatile metal carbonyls and halides with reactive gases.

4) Synthesis of molybdenum nitride compounds by thermal and photolytic decomposition of a molecular molybdenum azide compound ("$MoNN_3Py$").

Approach 1

The focus of this approach is to prepare organometallic molecules possessing the proper stoichiometry of molybdenum, co-metal (Co, Fe, Ni) and sulfur, which can be thermally decomposed to yield refractory materials suitable for HAS catalysis. Typically, metal oxides, sulfides and nitrides are produced by reacting the elements and/or reactive gases (after grinding the powders together) at high temperatures (800-1000°C) to produce thermodynamically stable phases. Through the use of organometallic precursors, the metals and sulfur are mixed on a molecular level before heating and do not require the high temperatures needed in conventional processing to overcome long atomic diffusion distances. It is through the use of lower temperatures (200-400 °C) resulting from molecular mixing of elements, that metastable phases, unobtainable through conventional means, can be synthesized.

The following organometallic compounds are currently being synthesized: $Cp_2Mo_2Fe_2S_2(CO)_8$ ($Cp=C_5H_5$), $Cp_2Mo_2Co_2S_3(CO)_4$, $(NEt_4)_2\{M(SPh)_4[Mo(CO)_4]_2\}$ (M=Ni,Co) $Cp^*_2Mo_2Co_2S_4(CO)_2$ ($Cp^* = C_5Me_5$), $Cp_2Mo_2Fe_2S_4(CO)_6$.

a) $Cp_2Mo_2Fe_2S_2(CO)_8$. This compound can be synthesized according to the following reaction:

$$Cp_2Fe_2S_2(CO)_6 + Cp_2Mo_2(CO)_4 \longrightarrow Cp_2Mo_2Fe_2(CO)_8 + 2CO$$

Both $Cp_2Fe_2S_2(CO)_6$ and $Cp_2Mo_2(CO)4$ the have been synthesized and characterized. More of the iron reactant is being synthesized in order to prepare approximately 3 grams of $Cp_2Mo_2Fe_2(CO)_8$.

b) $Cp_2Mo_2Co_2S_3(CO)_4$. The final reaction to produce this compound is:

$$Cp_2Mo_2(\mu\text{-}S)_2(\mu\text{-}SH)_2 + Co_2(CO)_8 \longrightarrow Cp_2Mo_2Co_2S_3(CO)_4 + 4CO$$

$Co_2(CO)_8Cp_2$ has been purchased and $Mo_2(\mu\text{-}S)_2(\mu\text{-}SH)_2$ is being synthesized.

c) $(NEt_4)_2\{M(SPh)_4[Mo(CO)_4]_2\}$ (M=Ni,Co). The general reaction yielding these compounds is:

$$(Et_4N)_2M(SPh)_4 + 2\ Mo(CO)_4C_7H_8 \longrightarrow (NEt_4)_2\{M(SPh)_4[Mo(CO)_4]_2\}$$

For this reaction, we have synthesized and characterized each of the precursors for both the cobalt and nickel reactions. We are in the process of purifying $(Et_4N)_2Ni(SPh)_4$ and $Mo(CO)_4C_7H_8$.

d) $Cp_2Mo_2Co_2S_4(CO)_2$. The synthesis of this compound is accomplished according to the reaction:

$$(C_5Me_5)_2Mo_2(S_2)S_2 + Co_2(CO)_8 \longrightarrow Cp_2Mo_2Co_2S_4(CO)_2 + 6CO$$

Work has yet to begin on this synthesis.

e) $Cp_2Mo_2Fe_2S_4(CO)_6$. The reaction to produce this compound is:

$$Cp_2Mo_2(\mu\text{-}S)_2(\mu\text{-}SH)_2 + Fe_2(CO)_9 \longrightarrow Cp_2Mo_2Fe_2S_4(CO)_6 + 3CO$$

$Cp_2Mo_2(\mu\text{-}S)_2(\mu\text{-}SH)_2$ is being synthesized (see reaction b) and $Fe_2(CO)_9$ has been made in sufficient quantity.

A summer research assistant has helped with the preparation and characterization of the desired organometallic compounds. Reactions a-c, e are near completion. It is anticipated that $Cp_2Mo_2Fe_2(CO)_8$, $Cp_2Mo_2Co_2S_3(CO)_4$, $(NEt_4)_2\{M(SPh)_4[Mo(CO)_4]_2\}$ (M=Co, Ni), $Cp_2Mo_2Co_2S_4(CO)_2$, $Cp_2Mo_2Fe_2S_4(CO)_6$ will be available within the next month. These heterobimetallic compounds will then be decomposed thermally. An evacuable Netzsch TG/DTA with a Quadrapole mass spectrometer attachment is being modified for use. This Netszch instrument will allow us to evaluate the thermal decomposition pathways of these organometallic compounds and thereby aid our efforts to identify the refractory products of decomposition.

Approach 2

Schrader et. al.[1] have demonstrated that conventionally prepared Chevrel phase materials are active toward HDS of thiophene. Through their research, it was observed that all of the materials exhibited some degree of activity, the compounds containing the larger cations (e.g., Ho, Pb) generated the highest HDS rate.

Approach 2 is divided into two parts. In the first part, refractory Chevrel phase materials will be synthesized using high temperature reactions (800-1200°C) in which the cation will be varied to include large cations (Ho, Gd, Pb, Sn), intermediate cations (Ag, In) and small cations (Co, Fe, Ni, Cu). Each will be evaluated for its catalytic nature relative to HAS. In the second part of approach 2, supported chevrel phase materials will be prepared; first with copper as the ternary metal according to syntheses reported by Sergent et. al.[2] and then attempts will be made to prepare supported Chevrel phases with larger cations. Currently, the reagents for the Chevrel phase syntheses are being obtained. The molybdenum compounds for preparation of supported Chevrel phase catalysts have already been prepared (see QTPR6, April 1993).

Approach 3

In addition to the large reactor illustrated in the previous quarterly report, a smaller reactor has been designed and completed for preliminary evaluations. Two reactions have been completed using the large reactor. In the second of these reactions, the product obtained from the reaction of gaseous $Mo(CO)_6$ and NH_3 at 800 °C was analyzed by BET and scanning electron microscopy to determine surface area and particle size. The surface area was determined to be 9.6 m^2/g by BET. Based on a packing density of 0.1 (volume occupied vs. total volume) and a weight density of 1.0 g/cm^3 the particle size would be 30 nm. While it is not possible to positively collaborate this particle size using the SEM, micrographs of representative grains indicate a particle size much smaller than a micron. From the micrographs, the surface morphology resembles a sponge in appearance. Energy Dispersive Spectroscopy, using the SEM, indicated molybdenum was the primary element in the material. No oxygen or nitrogen was observed in the EDS spectrum. As a result of these preliminary experiments, it appears that material comprised of relatively small particles can be made using this vapor phase reaction method.

Current work is underway to evaluate the influence of furnace temperature and reactant temperature (temperature applied to sublime the $Mo(CO)_6$) on particle size and morphology. In addition, material particle size and composition will be evaluated as a function of reactive and inert gas flow rates. Ultimately, the materials produced from these experiments will be evaluated for their catalytic ability, as the catalytic reactors become available.

Approach 4

As reported in preceeding quarterly report, a molybdenum azide compound, "$MoNN_3Py$", can be thermally decomposed into a molybdenum nitride refractory material through a gas evolving reaction. The particle size of this material is relatively low (0.5 to 1.5 m^2/g, using the BET method). The low surface area probably resulted from an annealing step following thermal decomposition of the azide.

As a supplement to the thermal decomposition study, we have attempted to decompose photolytically the molybdenum azide compound. The azide was dissolved in pyridine and placed in a quartz tube reactor containing a mercury lamp with a maximum output of 450 Watts. The azide solution was irradiated for 48 hours at maximum intensity. After the photolysis, the solvent was distilled from the solid and the solid was analyzed by FTIR and found to contain azide stretching modes, similar to the material before irradiation. Photolytic decomposition of this compound does not occur under the conditions outlined.

1.2.3 Transition Metal Oxide Catalyst Research

We have prepared a catalyst similar to those disclosed in U.S. Patent 4,943,551. Its molar composition is approximately 63% Cu, 18% Ce, 9% Zr and 10% K. The complete procedure for catalyst preparation is in Appendix 1.6.1.

We have not yet run any reaction tests or characterizations of this material. However, in the patent cited above, similar materials gave a carbon efficiency to alcohols of 98% and a rate to alcohols of 12 lbs/ft^3-hr, with 8% C_2^+ alcohols. In that study, carbon efficiency was defined as the fraction of the total CO converted to organic products which was converted to alcohols. The C_2^+ alcohols was defined as the fraction of alcohol product which was not methanol.

1.2.4 Reaction Engineering

During this reporting period we have devoted most of our modeling effort to the development of a packed-bed/membrane reactor model for conducting higher-alcohol synthesis reactions. The reactor configuration we have chosen to simulate has the potential of greatly enhanced performance for carrying out catalytic higher-alcohol synthesis reactions, when compared to the conventional packed-bed reactors.

A schematic representation of the packed-bed/membrane reactor is given in Figure 1.1, where the catalysts for higher-alcohol synthesis are packed inside an inorganic membrane tube permeable to hydrogen, carbon monoxide, carbon dioxide and water vapor, which in turn is housed inside an empty tube impermeable to all gases. For the purpose of this simulation, the inner membrane tube is assumed to be fully packed with K2O-promoted Zn-Cr oxide catalysts following the example of Tronconi et al[3]. A simplified reaction scheme of this catalyst consistent with the Tronconi

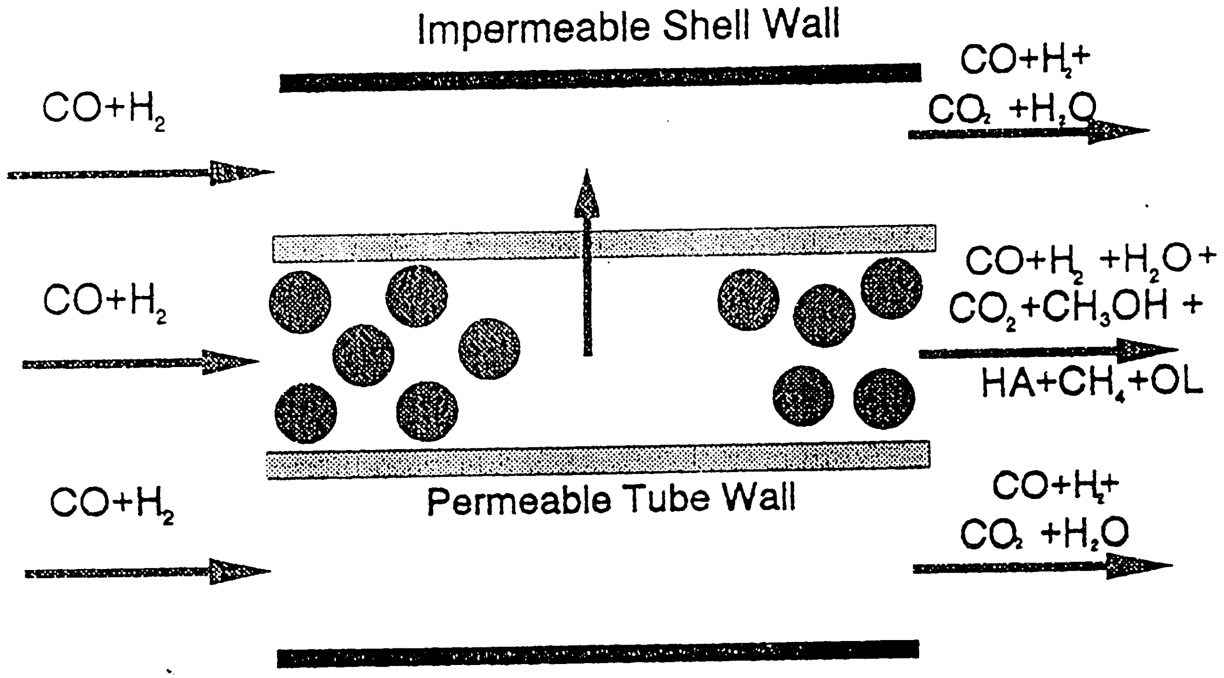

Figure 1.1 Schematic Representation of Catalytic Packed-Bed/Membrane Reactor

model was presented in a previous quarterly report (TPR6, Table 1.2) and used for modelling three types of ideal reactors.

According to this reaction scheme, water vapor strongly inhibits the rate of formation of higher alcohols (HA). The inhibiting effect of water was also reported by Frohlich and Cryder[4] and Smith and Anderson[5]. If operated properly, our proposed catalytic packed-bed/membrane reactor, as illustrated in Figure 1.1, can preferentially remove the water from the inner packed-bed reactor, thus enhancing the conversion to higher alcohols. This can be done by feeding hydrogen and carbon monoxide to both packed-bed and shell sides of the reactor, while maintaining the partial pressures of hydrogen and carbon dioxide in the shell to be higher than that inside the catalyst-packed tube to allow one-way permeation of both gases from shell to tube side. The latter is possible, since the key reactants, hydrogen and carbon monoxide, are consumed inside the packed-bed tubular reactor and hence their partial pressures in the tube side always decrease monotonically along the axial direction of the bed. The hydrogen and carbon monoxide passing through the shell side not only supply the needed reactants throughout the whole length of the packed-bed, but also carry away the unwanted carbon dioxide and the inhibitory water vapor, both permeating through the membrane out of the packed-bed due to transmembrane partial pressure gradients. At the reactor outlet, the water vapor can be condensed, the carbon dioxide separated, and the hydrogen and carbon monoxide recycled for reuse.

The purpose of this modelling effort is to investigate via numerical simulation whether the reactor configuration described above can lead to better higher-alcohols production.

We have developed a mathematical model for the catalytic packed-bed/membrane reactor described above and a computer program for solving the differential equations of the model. Numerical simulations conducted so far confirm that the proposed reactor system can indeed lead to enhanced reactor performance.

The ordinary differential equations (ODEs) used to model the packed-bed/membrane reactor, operating under isothermal and steady-state operation, are listed in Table 1.1. The notation used is defined in Table 1.2. A pseudo-homogeneous assumption is adopted for the inner packed-bed reactor, and plug flows with negligible axial and radial dispersions are assumed in both packed-bed and shell sides. A computer program PBMR1 was developed to solve the 12 initial-value type ODEs using LSODE, a stiff ODE solver[6]. During the development of the FORTRAN program, two different versions of LSODE (with and without involving the use of explicit expressions for Jacobian) were used to double check the program and the numerical results obtained.

Table 1.1

Mathematical Model for Catalytic Packed-Bed/Membrane Reactor

(A=CO, B=H_2, C=CH_3OH, D=HA, E=H_2O, F=CH_4,G=CO_2,H=OL)

Tube side

$$\frac{dN_A}{dz}+r_1+\alpha r_2+r_3+r_4+\frac{2K_A(P_A-P'_A)}{R_1}=0 \quad , \qquad N_A(0)=N_{A0} \qquad (1)$$

$$\frac{dN_B}{dz}+2r_1+2\alpha r_2-r_3+3r_4+\frac{2K_B(P_B-P'_B)}{R_1}=0 \quad , \qquad N_B(0)=N_{B0} \qquad (2)$$

$$\frac{dN_C}{dz}-r_1+r_2=0 \quad , \qquad N_C(0)=0 \qquad (3)$$

$$\frac{dN_D}{dz}-r_2+r_5=0 \quad , \qquad N_D(0)=0 \qquad (4)$$

$$\frac{dN_E}{dz}-\alpha r_2+r_3-r_4-r_5+\frac{2K_E(P_E-P'_E)}{R_1}=0 \quad , \qquad N_E(0)=0 \qquad (5)$$

$$\frac{dN_F}{dz}-r_4=0 \quad , \qquad N_F(0)=0 \qquad (6)$$

$$\frac{dN_G}{dz}-r_3+\frac{2K_G(P_G-P'_G)}{R_1}=0 \quad , \qquad N_G(0)=0 \qquad (7)$$

$$\frac{dN_H}{dz}-r_5=0 \quad , \qquad N_H(0)=0 \qquad (8)$$

Shell Side

$$\frac{dN'_A}{dz}-\frac{2R_1K_A(P_A-P'_A)}{R^2_2-R^2_1}=0 \quad , \qquad N'_A(0)=N'_{A0} \qquad (9)$$

Table 1.1 Continued

$$\frac{dN'_B}{dz}-\frac{2R_1K_B(P_B-P'_B)}{R^2{}_2-R^2{}_1}=0 \quad , \qquad N'_B(0)=N'_{B0} \qquad (10)$$

$$\frac{dN'_E}{dz}-\frac{2R_1K_E(P_E-P'_E)}{R^2{}_2-R^2{}_1}=0 \quad , \qquad N'_E(0)=0 \qquad (11)$$

$$\frac{dN'_G}{dz}-\frac{2R_1K_G(P_G-P'_G)}{R^2{}_2-R^2{}_1}=0 \quad , \qquad N'_G(0)=0 \qquad (12)$$

where

$$r_1=k_1(P_AP^2{}_B-\frac{P_C}{K_1}) \qquad (13)$$

$$r_2=k_2(\frac{P_C}{1+K_w\ P_E}) \qquad (14)$$

$$r_3=k_3(P_AP_E-\frac{P_GP_B}{K_3}) \qquad (15)$$

$$r_4=k_4P_B \qquad (16)$$

$$r_5=k_5(P_D)^{0.5} \qquad (17)$$

and

$$P_i=\frac{N_iS_cN_{T0}RT}{N_T\nu_0} \qquad (18)$$

Table 1.2

Notation and Parameter List

Notation

HA = pseudo higher alcohol with N_c carbon atoms
k_i = kinetic constant in rate expression for reaction i
K_i = effective permeability of component i
K_w = kinetic parameter associated with H_2O inhibition
N_c = average carbon number of HA
N_i = molar flux in axial direction (packed bed)
N'_i = molar flux in axial direction (shell side)
N_{io} = feed flux of component i
N_{TO} = total feed flux
N_T = total flux at any point z in the reactor
OL = pseudo olefin with N_c carbon atoms
P = total pressure
P_i = partial pressure of component i in the packed bed
P'_i = partial pressure of component i in the shell side
r_i = rate of reaction for reaction i
R = universal gas constant
R_1 = inside radius of membrane tube
R_2 = inside radius of reactor (shell side)
S_c = cross sectional area for flow
T = temperature
z = reactor length or axial distance from reactor inlet

Greek Letters

α = $N_c - 1$
ν_o = feed volumetric flowrate

Parameter Values Associated with Figures 1.2 through 1.5

$K_A = 2.198 \times 10^{-5}$ mol Pa^{-1} s^{-1} m^{-3}
$K_B = 5.875 \times 10^{-6}$ mol Pa^{-1} s^{-1} m^{-3}
$K_E = 1.762 \times 10^{-5}$ mol Pa^{-1} s^{-1} m^{-3}
$K_G = 2.576 \times 10^{-4}$ mol Pa^{-1} s^{-1} m^{-3}
$k_1 = 1.690 \times 10^{-18}$ mol m^{-3} s^{-1} Pa^{-3}
$k_2 = 1.200 \times 10^{-5}$ mol m^{-3} s^{-1} Pa^{-1}
$k_3 = 5.160 \times 10^{-11}$ mol m^{-3} s^{-1} Pa^{-2}
$k_4 = 4.010 \times 10^{-8}$ mol m^{-3} s^{-1} Pa^{-1}
$k_5 = 1.250 \times 10^{-3}$ mol m^{-3} s^{-1} $Pa^{-0.5}$
$K_1 = 1.539 \times 10^{-15}$ Pa^{-2}
$K_3 = 14.8$
$K_w = 8.752 \times 10^{-5}$ Pa^{-1}
P = 87 atm
T = 673 K
R_1 = 0.25 cm
R_2 = 0.75 cm

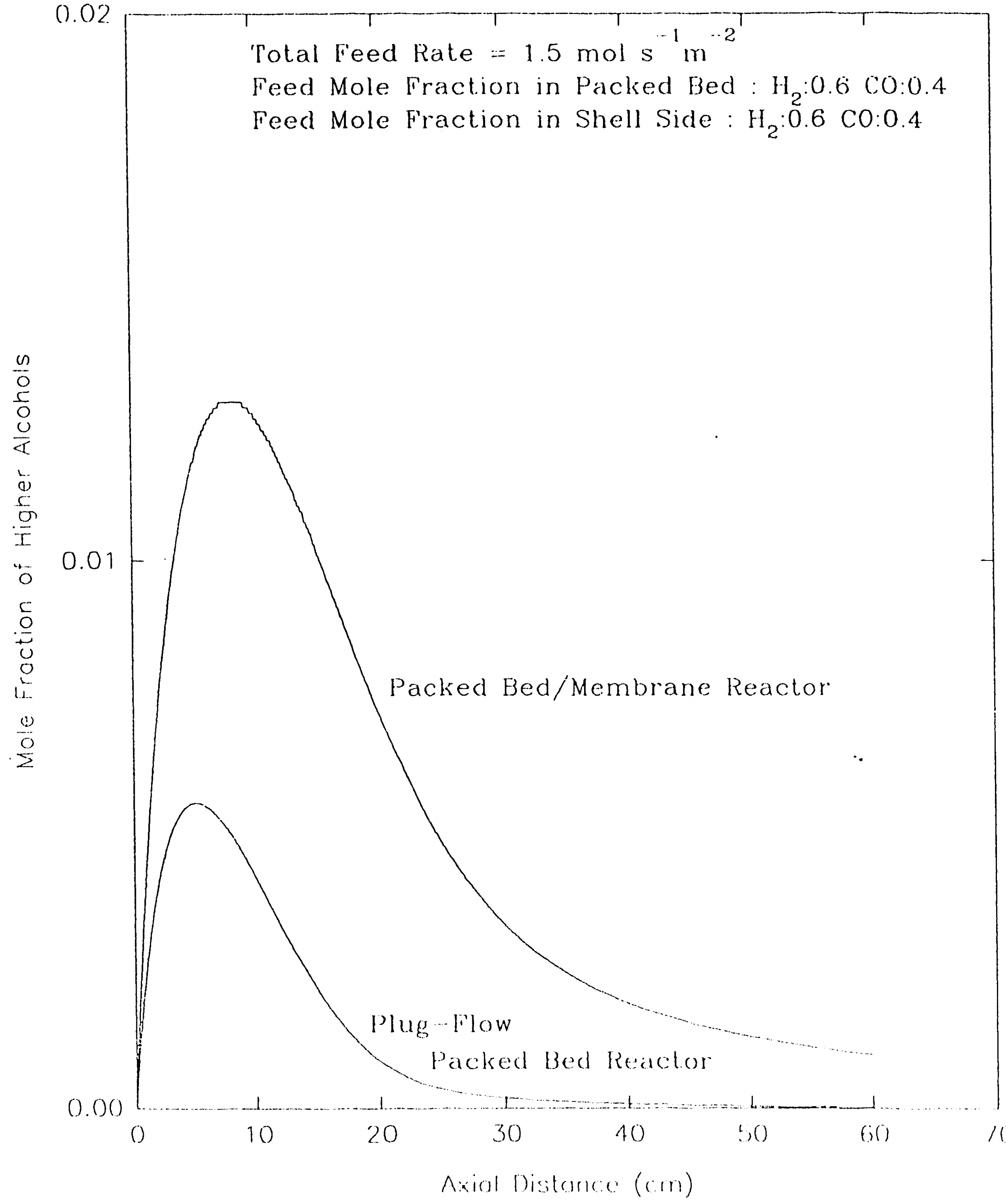

Figure 1.2. Comparison of Higher Alcohols Production in Packed Bed/Membrane Reactor and Plug-Flow Packed-Bed Reactor (Without Membrane)

Shown in Figure 1.2 are the results of one of the several simulation runs we have conducted so far. As can be seen from the diagram, when compared to an equivalent plug-flow packed-bed reactor, more than two- fold increase in the production of higher alcohols could be achieved by using the packed-bed/membrane reactor. For this simulation run, the steady-state concentration profiles of all the species in both packed- bed and shell sides of the packed-bed/membrane reactor are illustrated in Figures 1.3 through 1.5. The parameter values associated with this run are listed in Table 1.2. The driving force for the removal of inhibitory water vapor from the packed catalysts, i.e., the transmembrane partial pressure gradient of water, is clearly shown in Figure 1.3. Similarly, illustrated in Figures 1.4 and 1.5 are the driving forces for the permeation of hydrogen and carbon monoxide from shell to tube side and for the permeation of carbon dioxide from tube to shell side.

As long as the inhibitory effect of water vapor is also observed for the catalysts being developed in this project, the catalytic packed-bed/membrane reactor proposed, modelled, and simulated here has the potential of becoming one of the promising candidate reactors for catalytic higher-alcohol synthesis in the future.

1.3 Conclusions and Recommendations

Catalyst preparation and modeling are still at an early stage where preliminary hypotheses are being formed and tested. No conclusions are appropriate at this time.

1.4 Future Plans

Reactor unit construction at WVU is expected to be complete in the next quarter with initial results from standard catalyst testing. The reactor laboratory measurements at UCC&P were about to begin in early July, prior analytical problems having been solved. Modeling work will continue to focus on the potential for new reactor designs.

1.5 Appendices for Task 1

1.5.1 Reference Catalyst Preparation

The preparation procedure for preparing the 63%Cu, 18%Ce, 9%Zr, 10%K reference catalyst is listed below.

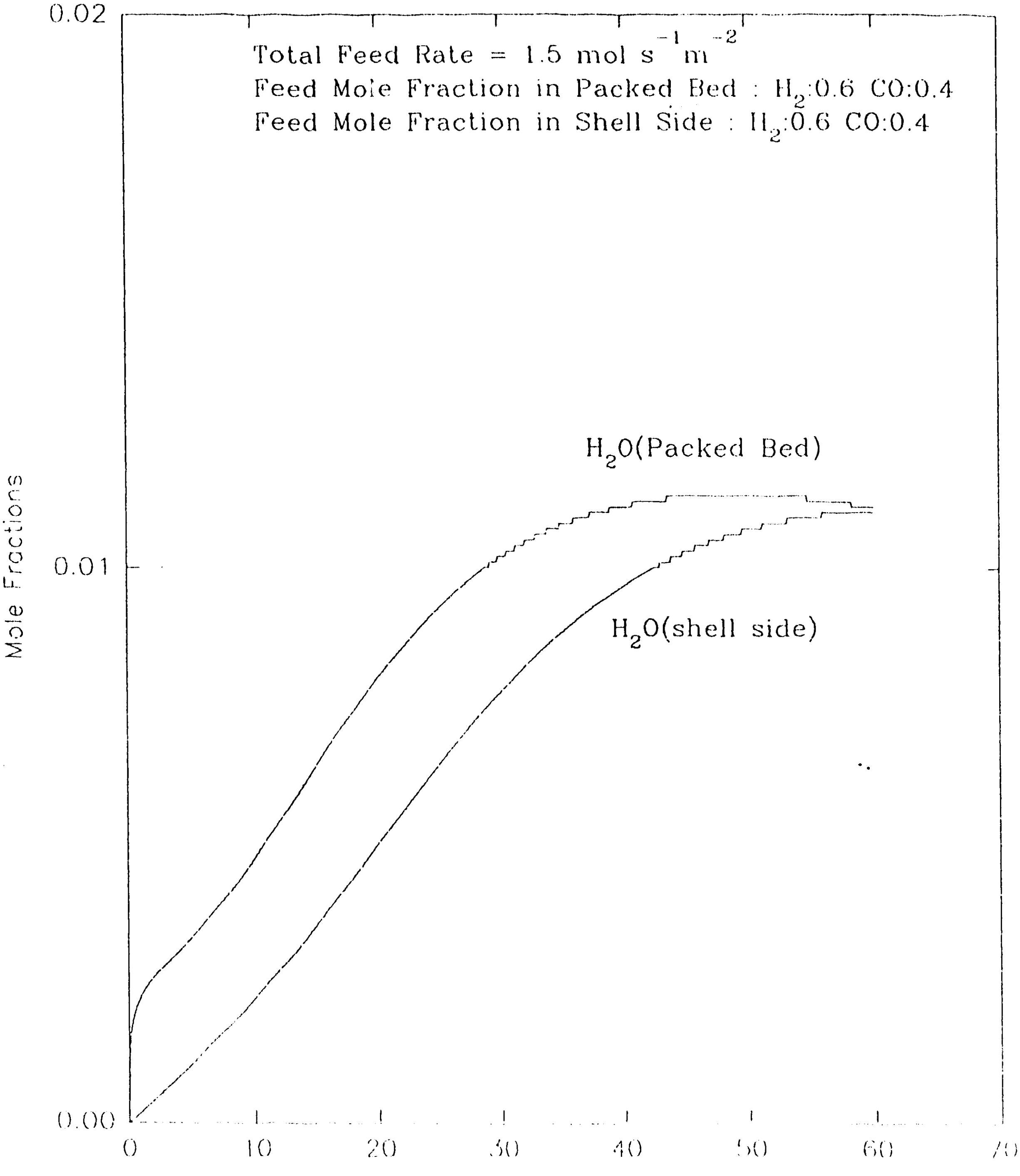

Figure 1.3 Concentration Profiles of Water Vapour in Catalytic Packed Bed /Membrane Reactor

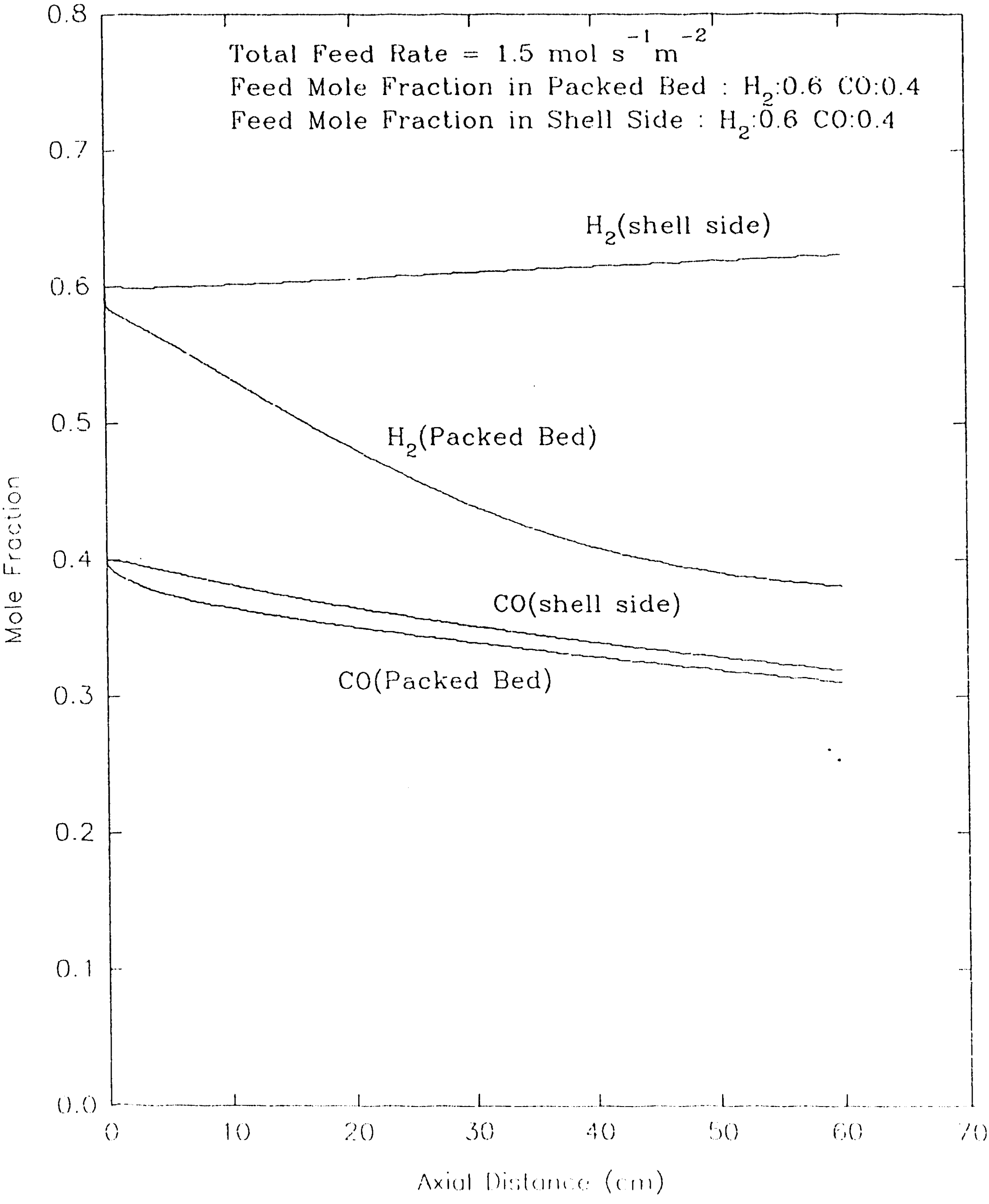

Figure 1.4 Concentration Profiles of Hydrogen and Carbon Monoxide in Catalytic Packed Bed /Membrane Reactor

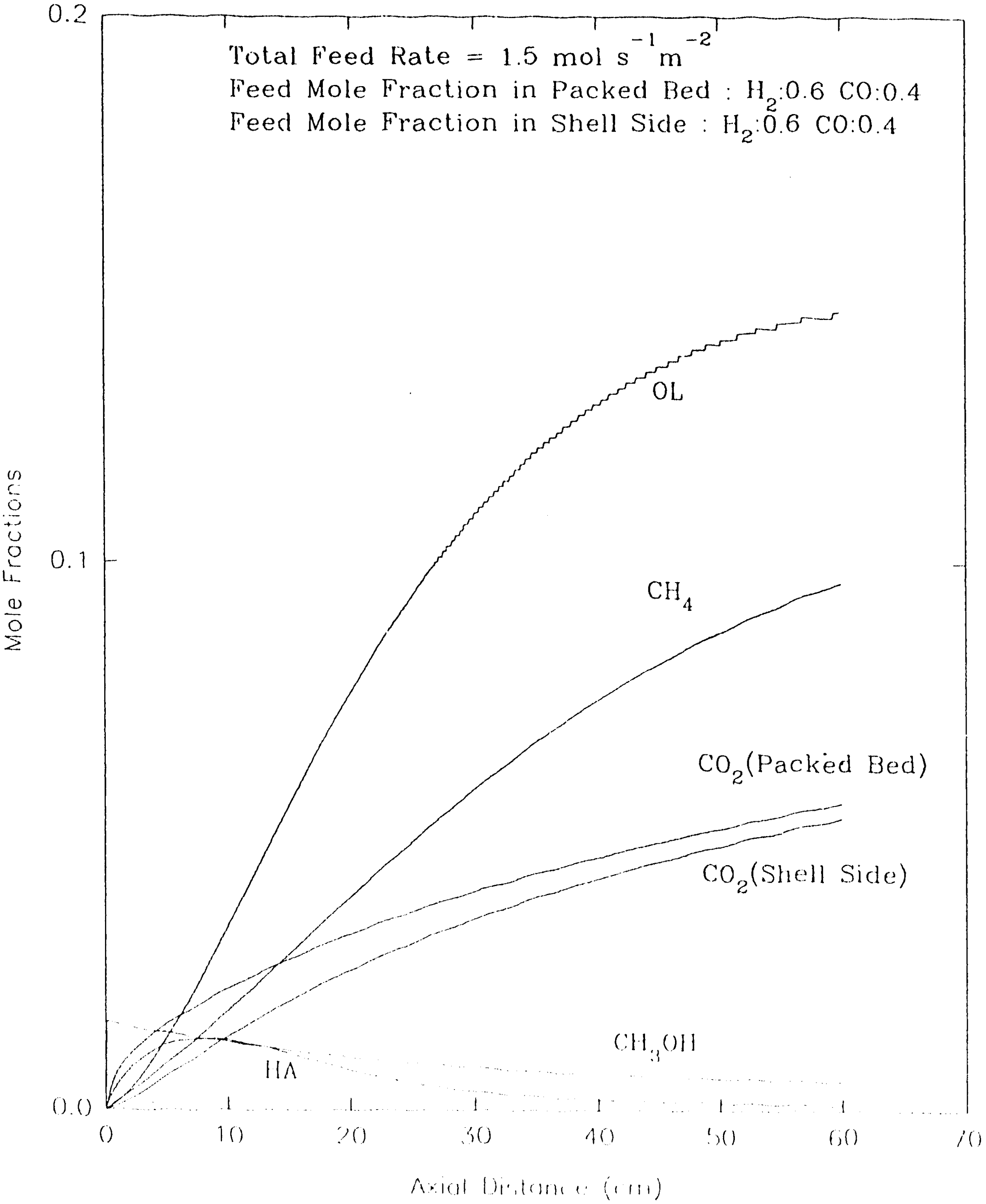

Figure 1.5 Concentration Profiles of Higher Alcohols, Methanol, Methane, Olefins, and Carbon Dioxide in Catalytic Packed Bed/Membrane Reactor

Day 1

Dissolve 15 g Na_2CO_3 in 50 ml of distilled water and then heat to 60°C.

In separate container, dissolve 15.46 g $Cu(NO_3)_2$-$3H_2O$ and 7.82 g $Ce(NO_3)_3$-$6H_2O$ in 100 ml distilled water.

Add (suspend) 1.11 g ZrO_2 (powdered) and heat solution to 60 °C.

Quickly add 60°C Na_2CO_3 solution to 60°C ZrO_2 suspension, keeping the ZrO_2 solution stirring, then stir 4 hrs while cooling to room temperature.

Collect precipitate on a filter and wash well with distilled water.

Dry overnight at 100°C.

Day 2

Calcine material at 400°C for 2 hrs, cool, then weigh.

Slowly add water to dry material until it no longer adsorbs water to determine the pore volume, then weigh to get the amount of water added. Let dry at 100°C overnight.

Day 3

Inpregnate with a solution of 0.98 g KOAc dissolved in an amount of water corresponding to the pore volume determined on Day 2.

Let dry overnight at 50°C.

Day 4

Calcine at 400°C for 2 hrs, then press into pellets or wafers.

Crush pellets and sieve to 30/40 mesh.

1.6 References for Task 1

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TASK 2. PROCESS SYNTHESIS AND FUEL EVALUATION.

2.1 Introduction

In previous quarterly reports, four base case designs for production of higher alcohol fuels from coal derived syngas have been presented. These were: (1) Texaco gasifier with natural gas, (2) Lurgi gasifier with natural gas, (3) Natural gas only, and (4) Texaco gasifier with sour gas shift converter. The natural gas or sour gas shift converter in cases 1, 2, and 4 were to alter the H_2 to CO ratio to the desired value of 1.1. Two additional base cases are under preparation, involving a Shell gasifier with natural gas and with a sour gas shift converter. In all four of these base cases, the alcohol synthesis reactor and alcohol separation section has been costed using values in similar designs. In order to facilitate optimization of this section of the process, a more detailed design is in progress.

An analysis of the current base cases has been under taken to determine if the economic status of the proposed alcohol fuels may benefit from economies of scale. This analysis was based on a literature review which suggested that plants of capacities substantially below 5000 metric tons/day are unlikely to be competitive for the bulk production of alcohols for fuel consumption or chemicals manufacture. The possibility of reducing the production cost of the mixed alcohol fuel product by taking advantage of economies of scale was briefly discussed in the First Quarter report for 1993. However, the effectiveness of this proposal was questionable due to uncertainty surrounding the scaling exponents for the gasifiers. Although questions still remain regarding proper scaling exponent for the gasifiers, attempts have been made to identify any constraints as well as any changes in economic feasibility that may be attributed to capacity changes by using generalized scaling exponents.

In terms of fuel evaluation and testing, work has focused on a) the corrosion effects of the esters in the alcohol blends, b) the maximum percentage of methanol that can be included in the alcohol blend and c) the effect of methanol and higher alcohols on the Reid Vapor Pressure (RVP) of the blends.

2.2 Accomplishments, Results and Discussion

2.2.1 Base Case Designs

Final economics for base cases involving the Shell gasifier have not been completed due to a lack of economic information on the gasification system. Two cases are being constructed, one with a sour gas shift converter after the gasifier, and one that uses natural gas to supplement the hydrogen lean gasifier outlet.

These cases are directly related to the Texaco gasifier base cases. The material balances for the Shell gasifier with sour gas shift is fairly close to that of the Texaco gasifier with sour gas shift. However, the Shell case with natural gas uses only half as much coal as does the Texaco case with natural gas. This is due to the very low H_2 to CO ratio from the Shell gasifier as compared to the Texaco.

2.2.2 Design and Optimization

In order to develop the procedure to optimize the entire coal to syngas to higher alcohols process, optimization of the syngas to higher alcohol portion of the process will be done first. In order to do this optimization, more detailed information regarding the alcohol synthesis reactor and the separation sequence is needed.

The alcohol synthesis reaction from syngas is a highly exothermic reaction. Therefore, the design of the reactor must provide for sufficient cooling so as to prevent runaway reactions. In our analysis, we consider the reactor to be isothermal heat exchanger type reactor in which the heat of the reaction is transferred to a boiling heat transfer fluid such as water. Any isothermal reactor design would be appropriate as long as sufficient heat transfer capability is provided. The reactor which is considered appropriate for this project has catalyst on the shell side and the cooler feed water on the tube side. The reactors with catalyst in the shell side are economically advantageous in comparison with the catalyst in the tube side because they minimize the shell diameter required to conduct a reaction. This is achieved by minimizing the amount of volume occupied by the coolant. There is greater difficulty in changing the catalyst and the frequency of catalyst addition and removal can be a major factor in choosing between the catalyst in shell and catalyst in tube reactors. For the present case the frequency of catalyst changes is such that catalyst in shell type reactors are appropriate. Catalyst in shell side also create mechanical and construction problems such as the number of tubes required and supporting the tube bundle. The size of the tube is chosen in such a manner that the volume occupied by it is minimized, thereby maximizing the area. However, the tube should be large enough so that the coolant fluid can be circulated in an appropriate manner. The tube thickness should also be such that it can withstand high enough pressures required for the reaction.

As an example, the design of an appropriate reactor for Base Case 1 is presented along with the design of the maximum size of reactor that can be built.

Data Provided	*Base Case 1*	*Maximum Size*
Heat Generation Rate	137.3 MW	205.1 MW
Feed Rate	351.93 Mkg/hr	525.71 Mkg/hr
Alcohols Production Rate	62.56 Mkg/hr	93.45 Mkg/hr
Catalyst Productivity	0.089 kg/s-m^3	0.089 kg/s-m^3
Pressure	136 atm	136 atm
Reaction Temperature	310°C	310°C

The following dimensions are fixed for both the reactors.

Catalyst Bed Length	15.24 m
Tube ID	0.025 m
Tube OD	0.0167 m
Tube BWG	8
Tube Material	Stainless Steel
Catalyst Pellet Diameter	0.00625 m
Catalyst Pellet Type	Sphere
Catalyst Bed Void Fraction	0.4
Average ΔT (Process - Steam)	15°C

The following are the dimensions obtained for the design of the reactor

Results	*Base Case 1*	*Maximum Size*
Inside Diameter of Reactor	5 m	6.1 m
Catalyst Bed Volume	195.1 m^3	291.4 m^3
Number of 50 ft. Tubes Required	13367	19966
Overall Heat Transfer Coefficients	563.3 W/m^2°C	498.1 W/m^2°C
Heat Transfer Area	16255 m^2	24281.1 m^2

The limitation on the size of the reactor is due to the problems encountered in fabricating and transporting the reactor. The upper limit on the size of the reactor is required when scale-up has to be considered. The capital cost of the reactor for Base Case 1 is $ 2.4 million while the capital cost for the maximum size reactor is $ 3.0 million. The cost data was made available by Union Carbide. The data available are for 1975 and the present cost is obtained by increasing the cost by appropriate multiplicative factor accounting for inflation, pressure factors and stress relief factor. The cost of the reactor does not include the cost for the catalyst.

The separation section will consist of a sequence of distillation columns. These columns will separate the stream coming out of the reactor into appropriate fuels alcohol blends. For the design of the distillation columns appropriate thermodynamic data is required to separate the methyl acetate and ethyl acetate which are present in very small quantities. Union

Carbide has provided the appropriate thermodynamic package which has been converted into ASPEN usable format from IPES. The data is being presently tested to obtain rigorous distillation column design along with the cost of the network of the column.

Simulated annealing will be used to generate the optimum cost of the reactor and separation system considered simultaneously. The optimization of the reactor or the separation unit by itself would not be appropriate as this might lead to an overall sub-optimal design.

2.2.3 Economics of Scale-up

In retrospect, current design capacities were only approximately 1500 metric tons/day which may partially explain their unfavorable economic status. Efforts were, therefore, undertaken to increase the capacities of these base cases in order to bring them into the feasible production realm suggested by the literature. A simple scaling exponent of 0.7 was applied to the installed fixed capital for each base case. All other factor were assumed to scale linearly. These scaling exponents were incorporated into the existing spreadsheet model providing a means of estimating the long run average cost curves for the respective base cases (Figures 2.1 & 2.2). Examination of these figures reveals that the process may benefit significantly by increasing the capacity of the current facility designs. However the extent to which the capacity can be increased may be limited by special factors such as regional coal supplies. Evidence of this is suggested in Figures 2.3 & 2.4 which illustrate demand for coal as a function of capacity.

For all practical purposes, regional coal markets, regardless of location, would have difficulty in sustaining the demand placed on them by a facility much larger than 1200 metric tons/day. This level of alcohol production would require a coal feed in the range of 6.5 to 9 million metric tons/year depending on the technology employed. To put this in perspective, consider that fact that the average coal fired power plant in the United States consumes a little more than 2.5 million metric tons of coal a year. The potential of handling problems associated with such large quantities may need to be addressed in the future. However, there are a few large coal fire power plants in the United States that consume volumes of coal equivalent to the amount of the proposed alcohol fuel plant. Therefore, it is reasonable to assume that the coal handling and acquisition practices employed by these facilities could be applied to the proposed alcohol fuel plant.

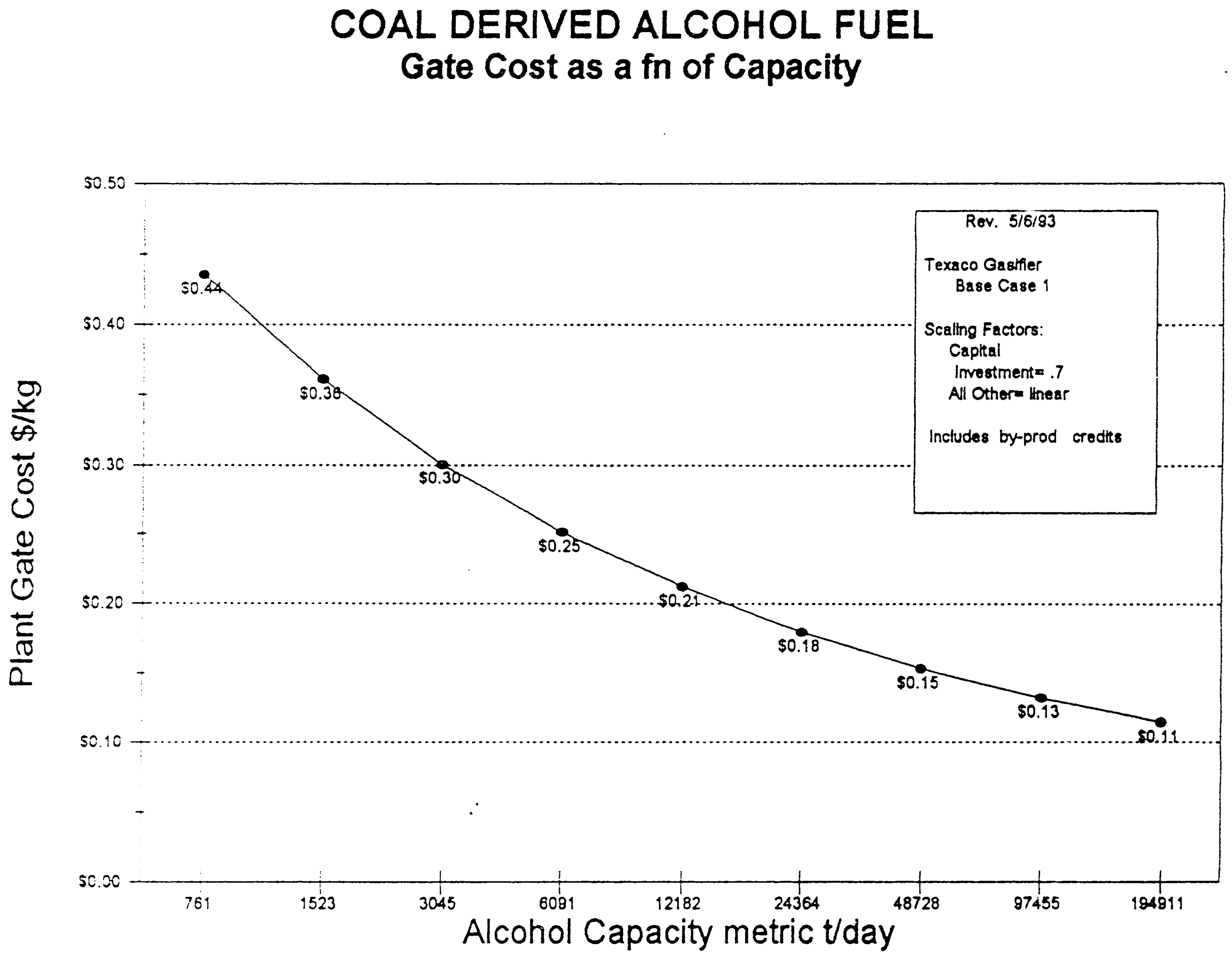
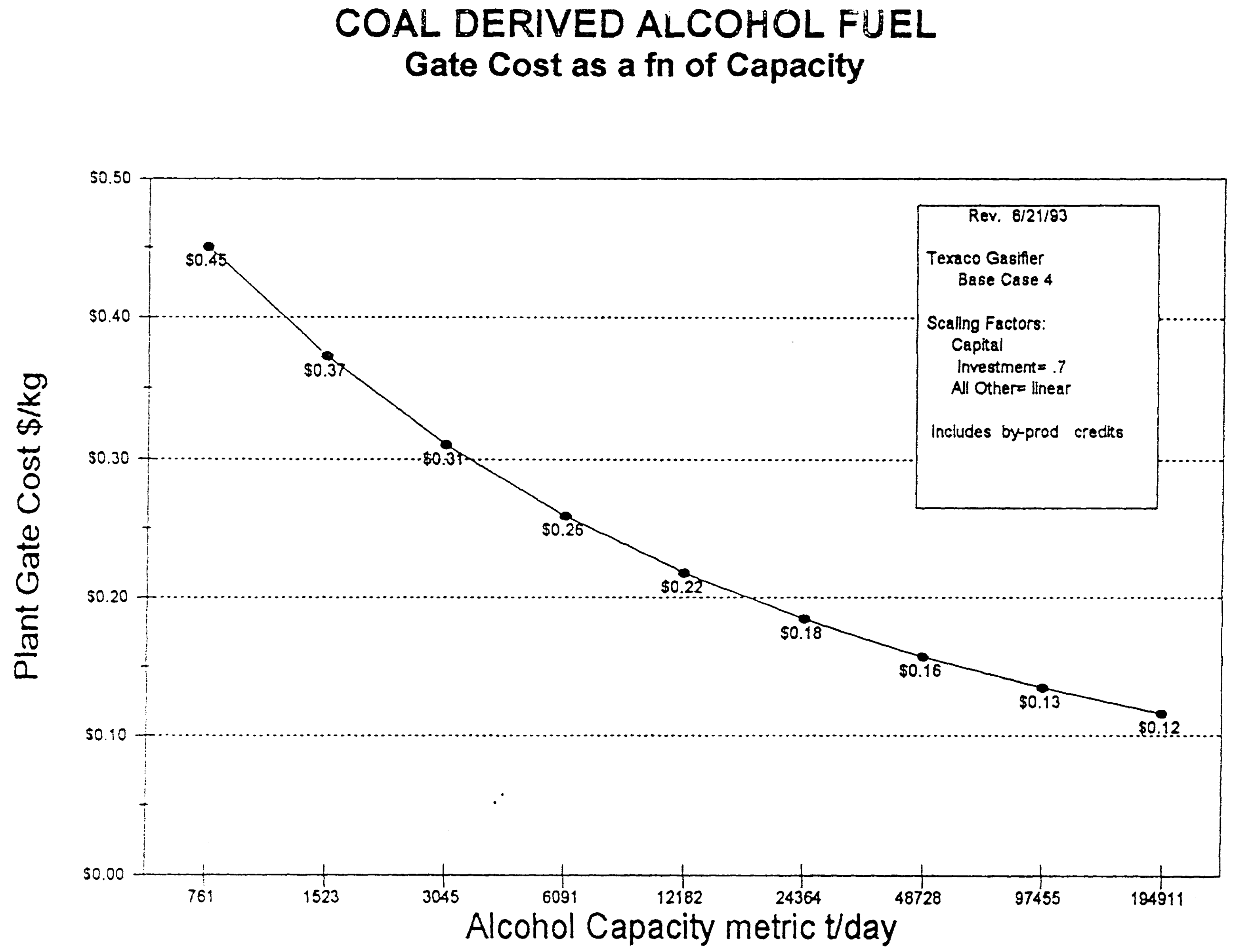

COAL DERIVED ALCOHOL FUEL
Gate Cost as a fn of Capacity
Plant Gate Cost $/kg
$0.50
$0.40
$0.30
$0.20
$0.10
$0.00
Alcohol Capacity metric t/day
761
1523
3045
6091
12182
24364
48728
97455
194911
$0.44
$0.36
$0.30
$0.25
$0.21
$0.18
$0.15
$0.13
$0.11
Rev. 5/6/93
Texaco Gasifier
Base Case 1
Scaling Factors:
Capital
Investment= .7
All Other= linear
Includes by-prod credits

Figure 2.1



COAL DERIVED ALCOHOL FUEL
Gate Cost as a fn of Capacity

Figure 2.2

COAL DERIVED ALCOHOL FUEL

Coal Consumption as a fn of Capacity

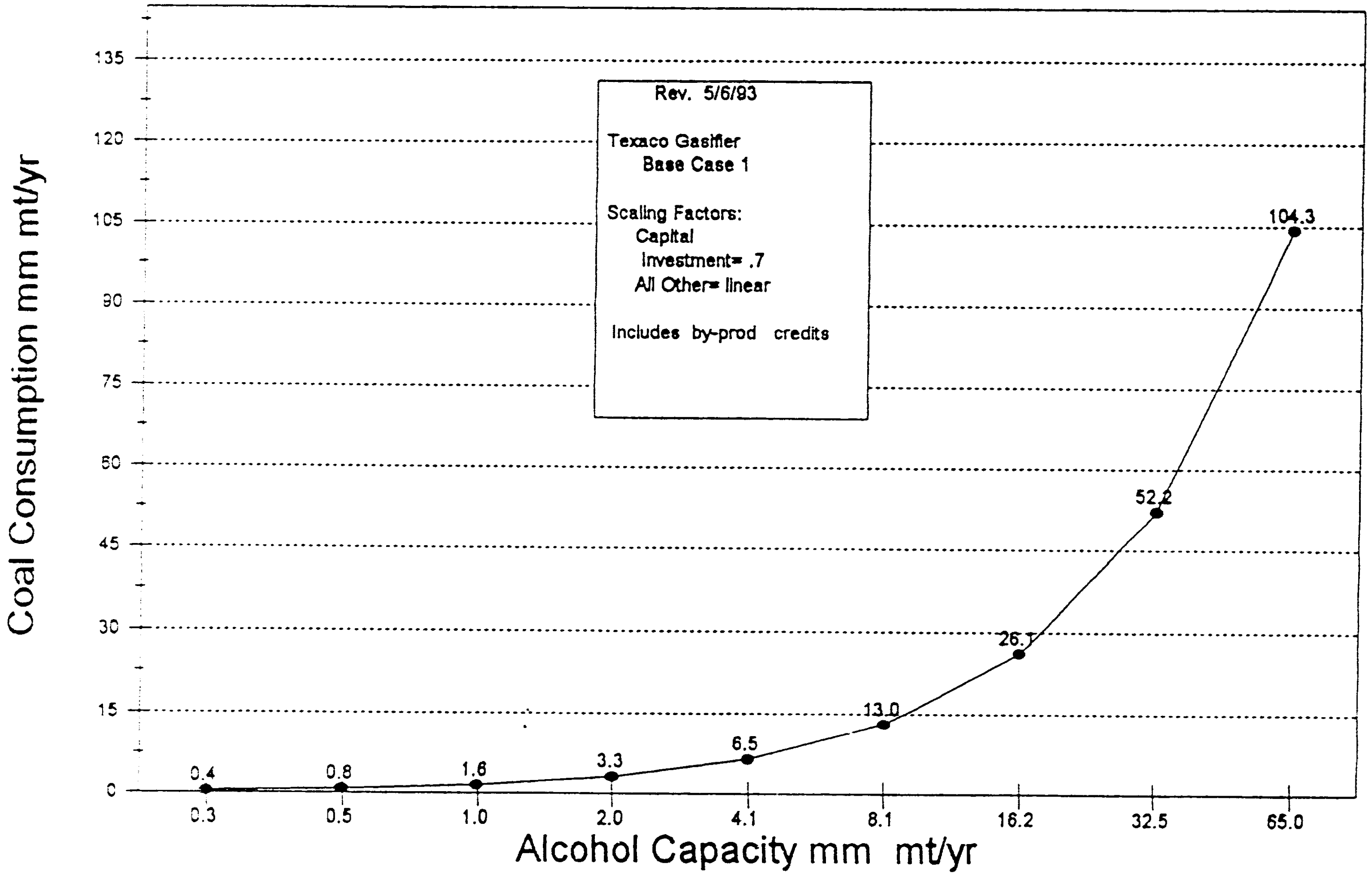


Figure 2.3

COAL DERIVED ALCOHOL FUEL
Coal Consumption as a fn of Capacity

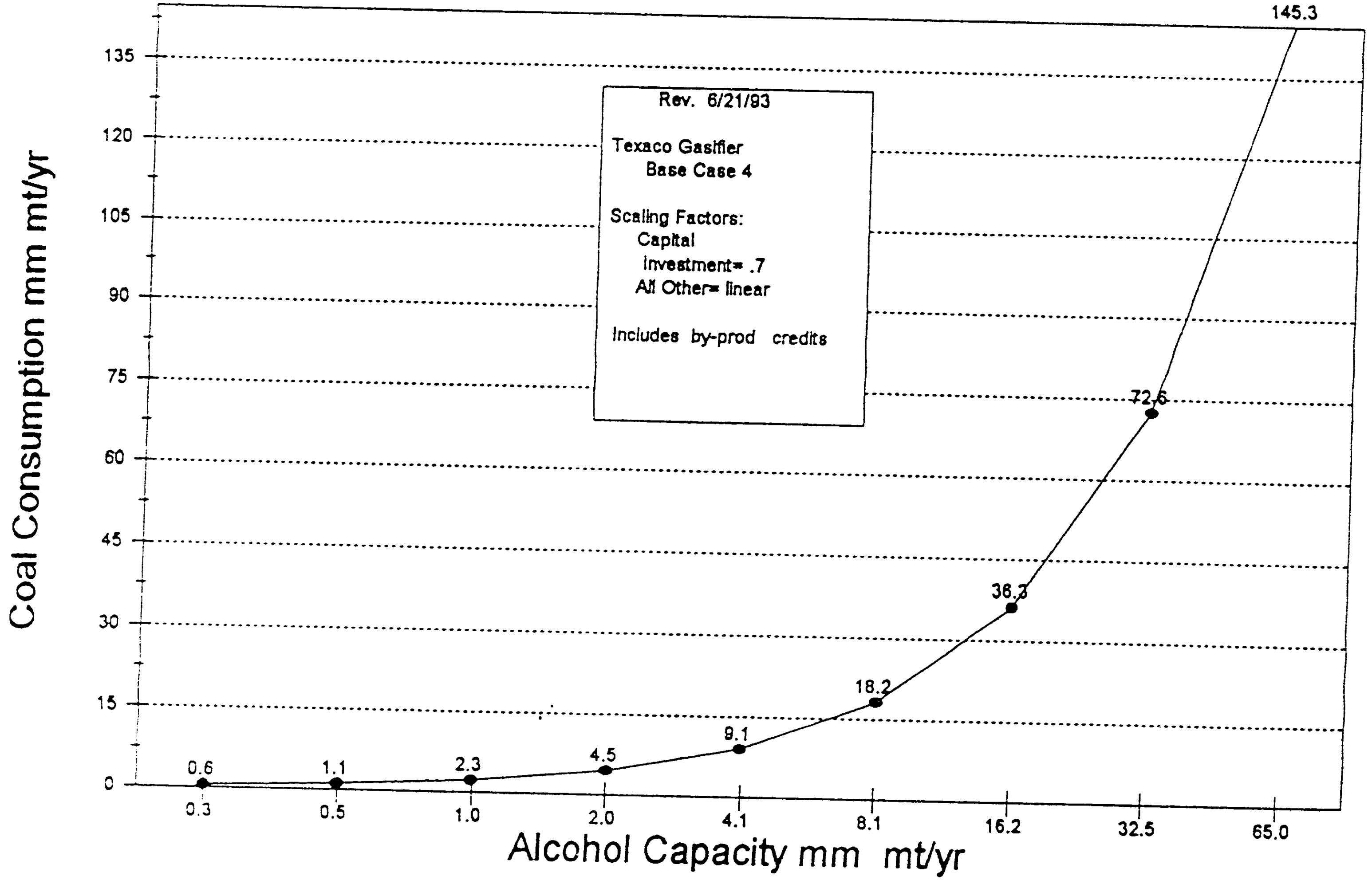


Figure 2.4

COMPOSITION OF THE ALCOHOL MIX PRODUCED BY THE MOLY-SULFIDE CATALYST.

Constituents (Mol. wt.)	% by lb moles	% by weight
Methanol (32)	41.6	30.76
Ethanol (46)	43.4	46.13
Propanol (60)	9.61	13.32
Butanol (74)	2.42	4.14
Pentanol (88)	1.00	2.03
Methyl acetate (74)	1.18	2.02
Ethyl acetate (88)	0.79	1.61

Table 2.1

2.2.4 Environmental Considerations

In order to construct a plant such as the one being designed here, current environmental regulations must be followed. Therefore, a preliminary environmental analysis of the sulfur removal portion of Base Case 1 has been completed. This includes fugitive emissions and stack emissions. The detailed results are found in Appendix 1. The results indicate that for SO_x compounds, there should be no trouble meeting environmental regulations. However, for H_2S containing compounds and for ozone, the process would be over the threshold values. This requires application of BACT (Best Available Control Technology) which could significantly increase the cost of construction and operation of a coal to syngas to higher alcohols process.

2.2.5 Fuel Evaluation

2.2.6 Corrosion Effects

The alcohol mixture synthesized using the moly-sulfide will contain small quantities of methyl acetate and ethyl acetate. These two esters will hydrolyze to form acetic acid and propionic acid which are potential corrosive agents. The composition of the gasoline-alcohol blend that would be formed is shown in Table 2.1. It is evident that although the quantity of esters present in the blend is rather small, compared to the alcohols, an extensive literature review was conducted to assess the potential corrosion problems that these esters could pose for the fuel tanks, the fuel distribution system and the combustion chamber.

Stoichiometry of the hydrolysis reactions, Equations 2.1 and 2.2, show that in a 100 lb moles of the alcohol mix, 1.18 lb moles of acetic acid (Molecular Wt.= 60) and 0.79 lb moles of propionic acid (Molecular Wt.= 74) would be formed, assuming complete hydrolysis. Also, as a result of these hydrolysis reactions, an additional methanol in the amount of (1.18 + 0.79) lb moles is formed.

$$CH_3\text{-}CO\text{-}OCH_3 + HOH \longleftrightarrow CH_3\text{-}CO\text{-}OH + CH_3OH$$

Methyl Acetate   Acetic Acid

(2.1)

$$C_2H_5\text{-}CO\text{-}OCH_3 + HOH \longleftrightarrow C_2H_5\text{-}CO\text{-}OH + CH_3OH$$

Ethyl Acetate   Propionic Acid

(2.2)

Thus, the net weight percentage of acetic acid in the alcohol mixture (after hydrolysis) is

1.18*60*100%/(41.6*32+43.4*46+9.61*60+2.42*74+1.00*88+1.97*32
+1.18*60+0.79*74) = 1.65%

The net weight percentage of Propionic acid in the alcohol mixture (after hydrolysis) is

0.79*74*100%/(41.6*32+43.4*46+9.61*60+2.42*74+1.00*88+1.97*32
+1.18*60+0.79*74) = 1.10%

When the alcohol mixture is blended with gasoline to make a gasoline-alcohol blend of 80% gasoline, 20% alcohols, the concentrations of acetic and propionic acids are reduced to 0.33% and 0.22% respectively. In fact, the acid concentrations are expected to be even lesser because the hydrolysis reaction does not go to completion. Because of the small concentrations of the organic acids, their corrosion effects should not be of much concern. The quantity of formic acid formed by the virtue of the alcohol combustion is far greater than that formed due to the hydrolysis of these esters. Nevertheless, the corrosion effects of the organic acids are summarized below.

In general, formic acid is not injurious to aluminum at any temperature. It catastrophically corrodes pure iron, C-steel and cast iron at all concentrations and temperatures. Stainless steel shows particular resistance to dilute (<5%) and concentrated (>80%) acid. However, even at 20°C, 10-70% acid corrodes SS. The rubber gaskets are also resistant to dilute acids.

Acetic acid does not corrode aluminum at 20-50°C (reduction of less than 2.5 gm/m^2/day). At the boiling point, corrosion is significant (60-120 gm/m^2/day). The vapors of acetic acid have virtually no effect on aluminum. Acetic acid is fairly compatible with pure iron, C-steel, stainless steel and cast iron. However, at temperatures near the boiling point temperature, SS is corroded badly.

The corrosion effects of Propionic acid are just the same as acetic acid.

Ryan, et al. (1981) showed that apart from the corrosive constituents that are formed by the hydrolysis of esters, there is a major corrosion problem by the combustion products of methanol and to a lesser degree of ethanol. Naegeli (1989) showed that a layer of liquid methanol ignited on a polished steel coupon produces a distinct rust residue. During combustion of methanol, small amounts of formic acid, formaldehyde and dioxymethylene peroxide (CH_2OH-OO-CH_2OH) are formed as partial oxidation products. Some percentage of these products comes back to the liquid layer by convection and gets dissolved. Formic acid was identified as the primary rust promoter by the investigator. Owens, et al. (1980) proposed three possible mechanisms listed below for the wear:

1. Methanol and partial combustion products attack metal directly because of corrosion.

2. The high latent heat of methanol and the high F/A ratio for methanol causes excessive accumulation of liquid methanol on the cylinder walls. This liquid methanol washes away the lubricant film from the surface, resulting in metal removal by adhesion and abrasion.

3. The methanol and its combustion products may interfere with the lubricant and/or the additive package.

Ichimiya, et al. (1985) confirmed the results of several other investigators who were trying to relate the extent of corrosion problem and the running temperature of the engine. Wear, as measured by the accumulation of iron in the lubricant, was most apparent when the engine coolant and lubricant temperatures were below 70°C. At higher temperatures, the wear characteristics of neat methanol approached that of unleaded gasoline. Baisley and Edwards (1981) concluded from their studies that another important factor which affects the corrosion rate is the mode of fuel injection into the combustion chamber. When vaporized methanol is fed into the combustion chamber (with enough degree of superheat to ensure that no condensation takes place), corrosion is less. With carbureted methanol, wear increases tremendously. Wear has been found to be inversely proportional to the cylinder wall temperature.

To counteract the corrosion problem of alcohol fuels, a lot of work has been done in formulating special fuel additives and lubricant additives which would prevent wear/corrosion associated with alcohol fuels. It has been seen that inhibitors can provide a reasonable protection against corrosion which otherwise could severely damage carburetor, fuel pump, fuel line, fuel filter, and fuel tank. Walker and Chance (1983) report in their studies that corrosion resistant materials could be used for making the engine parts. For example, GM do Brasil coats the carburetor with nickel and the fuel tank with tin. They also reported that acetic acid alone or in combination with ethyl acetate does not pose a severe corrosion problem in hydrated ethanol fuels. On the other hand, Cl^- ion, even in the concentration range of 10 ppm, had a synergistic effect in hydrated ethanol fuel with the other impurities. This combination causes corrosion many times greater than that caused by any single contaminant. Walker and

Chance (1983) used a variety of inhibitors in their study to protect mild steel. The only two inhibitors that gave exceptional results are a dimer acid type inhibitor (commonly used in pipelines) and a blend of glycols and amines (which is also sold in Brazil for addition to the fuel tank). It should be noted that the most effective use of an inhibitor would be to make sure that it is added to the fuel at the time of production.

A variety of tests have been performed by different investigators to see the effect of changing the lubricant composition on corrosion by oxygenated fuels/neat alcohols. Marbach, et al. (1983) reported that a magnesium based detergent additive in the baseline lubricant is less effective in protection against wear as compared to a calcium based additive. Ashless dispersant chemistry also plays an important part in the wear control. Additives are surface active agents which have a polar group at one end and an oleophilic/hydrophobic group at the other. The polar group attaches itself to a metal or other surface while the other group repels water and provides an oily layer to prevent rust from forming. A wide range of chemicals are used as anti corrosion additives including esters or amine salts of alkenyl succinic acids, alkyl orthophosphoric acids, alkyl phosphoric acids and aryl sulfonic acids. In the above study, a lubricant containing the following additives was used: calcium sulfonate detergent dispersant (provide detergency as well as neutralization for the acid), ashless phosphorus dispersant, alkyl zinc dithiophosphate (an acid neutralizer), a dispersant-type viscosity index improver (polymethacrylate), and an ashless inhibitor. All the additives were maintained at different concentrations in different runs of the test. It was seen that the ashless dispersant plays an important part in the lubricant formulation in combating methanol-related wear. The conclusion of Mg based additive being less effective than Ca based additive was derived by replacing calcium sulfonate detergent dispersant by magnesium sulfonate detergent dispersant.

Buck, et al. (1989) conducted lubrication studies to bring to the fore the additives approach of enhancing corrosion protection. A mineral oil (as the base product, let us call it Min-1) was spiked with highly alkaline additives to neutralize the formic acid formed. Min oil + a highly overbased metallic detergent (sulfated ash content of 1.5%), with the final total base number being 12, drastically reduced corrosion/wear. However, Min oil + a highly overbased ashless dispersant was not as effective even though it had the same final total base number (of 12). It was seen that even a poorly based metallic detergent provided outstanding protection, thus highlighting an important fact that although the oil alkalinity plays a very important part in acid neutralization, it is the kind of alkaline additive added that is critical. The surface affinity of the metallic detergents (repelling away all corrosives) is probably the reason for their protective action toward the cylinder.

2.2.7 Blend Composition

The use of additives - their composition and quantity, in unleaded gasoline is regulated by the EPA (Owen and Coley, 1990) which ensures that the subsequent tailpipe and evaporative emissions will not be affected. In the case of oxygenates, the EPA has ruled that aliphatic alcohols and glycols, ethers and polyethers may be added to the fuel provided that the amount of oxygen in the finished fuel does not exceed 2% wt. Methanol is excluded from this approval. This is known as the "substantially similar" ruling, as these components are considered to be substantially similar to fuels in widespread use before the requirement for EPA approval. A number of specific proposals have been granted waiver from the 2% wt. limit. e.g., 'Gasohol', a mixture of 10% vol. ethanol with gasoline has 3.7% wt. oxygen. A mixture of TBA and methanol can have a maximum of 3.7% wt. oxygen, provided that methanol does not form more than 50% of the mixture. Another waiver, which is called the "Dupont waiver" allows methanol up to 5% vol. plus at least 2.5% vol. cosolvent (ethanol, propanols or butanols) plus a corrosion inhibitor. The Dupont waiver also allows a maximum of 3.7% wt. oxygen.

A number of possible alcohol blends (MPHA) were determined based on the assumption that the limit of 3.7% wt. oxygen in the alcohol-gasoline blend would be applicable for us. Table 2.2

shows the weight % of oxygen in the various alcohols. By varying the percentages of C_1-C_4 alcohols, the wt. % of oxygen in the (10% alcohol-90% gasoline) blend is calculated as shown in Table 2.3.

2.2.8 Reid Vapor Pressure of Blends

From his extensive studies on the variation of Reid Vapor Pressure (RVP) of blends with the alcohol composition, Furey (1985) concluded that alcohols form non-ideal mixtures with gasoline. As such, the addition of certain alcohols such as methanol and ethanol produces blends which have higher vapor pressures than either the gasoline or alcohol alone. Moreover, the effect of alcohols on the RVP is not linear, and very small concentrations of alcohol in gasoline cause the most significant increase in RVP of the blend. Table 2.4 shows the RVP of gasoline and pure alcohols.

Table 2.5 shows the drastic increase in the RVP of pure gasoline when it is mixed with methanol and ethanol. It can be easily seen that tertiary butyl alcohol does not increase the RVP of the blend as drastically as methanol and ethanol.

The higher alcohols (such as TBA) mellow down the drastic

THE WEIGHT PERCENTAGE OF OXYGEN IN DIFFERENT ALCOHOLS

Alcohol (Mol. wt.)	Weight % of Oxygen
Methanol (32)	50
Ethanol (46)	34.78
Propanol (60)	26.67
Butanol (74)	21.62

Table 2.2

ALCOHOL-GASOLINE BLENDS (10% ALCOHOL)

Percent n-Butanol (Vol.%)	Percent Propanol (Vol.%)	Percent Ethanol (Vol.%)	Percent Methanol (Vol.%)	Total % Oxygen (by wt.)
5	2	3	0	2.66
5	1	4	0	2.74
5	1	3	1	2.89
5	2	1	2	2.96
5	1	1	3	3.19
5	0	1	4	3.43
5	1	0	4	3.35
4	2	1	3	3.25
4	1	2	3	3.32
4	0	1	5	3.71
4	1	0	5	3.63

Table 2.3

RVP (KPa) OF PURE GASOLINE AND ALCOHOLS

Component	Gasoline	Methanol	Ethanol	TBA
RVP (Kpa)	62.1	31.0	15.2	-

Table 2.4

EFFECT OF THE COMPOSITION OF DIFFERENT ALCOHOLS ON THE RVP (KPa) OF BLENDS

Conc. (Vol. %)	Methanol	Ethanol	TBA
0	62.1	62.1	62.1
2.5	83.6	-	63.1
5	84.8	69.6	62.7
7	-	-	62.7
10	85.5	69.0	62.4
15	84.8	68.3	-
20	84.1	67.2	-
30	83.1	65.5	-
50	78.6	60.2	-
70	69.0	48.3	-
90	49.6	29.6	-
100	31.0	15.2	-

Table 2.5

increase of RVP that occurs on the addition of methanol to gasoline. In Table 2.6, for clarity sake, the RVP of blends with pure methanol and 1:1 TBA/Methanol are shown for the same alcohol percentage.

Tables 2.5 and 2.6 clearly indicate that the blends become very volatile as compared to pure gasoline. This causes the total evaporative emission losses to go up and it is for this reason that higher alcohols like TBA have to be used as cosolvents. Since, in most of the commercial blends, the percentage of alcohols does not exceed 5%, Table 2.7 gives a better idea about the effect of alcohols on the RVP (in KPa) of commercial blends.

Some general conclusions could be drawn from Tables 2.5, 2.6 and 2.7. TBA in concentrations up to 10% has only a small effect on the vapor pressure of blend. However, lower alcohols cause a significant vapor pressure increase when added in small concentrations to gasoline. The RVP maxima for all the oxygenates occur at 5-10% oxygenate concentration. Moreover, the bulk of the RVP increase occurs at as little as 0.25% of methanol or ethanol.

The reason for the non-ideality of the gasoline-alcohol blends is that pure methanol exists as a cyclic tetramer with an effective molecular weight of 32*4=128. This is attributed to the strong H-bonding between the individual methanol molecules. As such, methanol behaves like a high molecular weight compound and consequently has a low vapor pressure. However, in a mixture with gasoline, which is highly non-polar, the H-bonds are weakened and consequently, the volatility goes up. The increase in volatility of the gasoline-alcohol blend, as a result of methanol addition, has direct implications on the blends produced in this project. The task of proving to the EPA, that the new blend is "substantially similar" to gasoline becomes more tedious. Hence, the percentage of methanol that can be added to the mix has to be studied very closely.

COMPARISON OF THE RVP (KPa) OF GASOLINE-METHANOL AND GASOLINE-1:1 TBA/METHANOL

Conc. (Vol. % of Alcohols)	Methanol	1:1 TBA/Methanol
0	62.1	62.1
2.5	83.6	-
5	84.8	78.3
7	-	-
10	85.5	78.3
15	84.8	77.6
20	84.1	76.5
30	83.1	73.8
50	78.6	68.3
70	69.0	57.6
90	49.6	38.6
100	31.0	24.1

Table 2.6

EFFECT OF ALCOHOLS ON THE RVP (KPa) OF BLENDS AT LOWER CONCENTRATIONS

Conc. (Vol. %)	Methanol	Ethanol	Gasoline grade TBA (GTBA)
0	80.8	80.8	80.8
0.25	87.7	83.4	-
0.5	91.0	86.9	81.7
1.0	96.9	91.0	82.1
2.0	101.4	94.5	-
5.0	103.1	95.8	84.5

Table 2.7

2.3 Conclusions

The preliminary results of this scale up procedure would indicate that the capacity of the current base cases should be increased by a factor of eight. This would yield annual production of 4.1 million metric tons and essentially reduce the plant gate cost by approximately 41 percent in both cases. A facility of this size would be the equivalent of a medium sized oil refinery and would be capable of sustaining local market demands as a fuel oxygenate (see Table 2.8). The actual competitiveness of this product with current oxygenates such as MTBE remains to be determined.

On a price basis alone, the mixed alcohol produced by this size facility appears to be competitive with MTBE. The plant gate cost for the mixed alcohol would be $0.21-$0.22/kg depending on the technology employed. MTBE on the other hand currently sells for approximately $0.36/kg. This would provide producers of the mixed alcohol a considerable margin for markup and transportation cost without jeopardizing the competitiveness of the product. However, price is only one determinant influencing the demand for blending agents. Other factor such as performance characteristics must be considered. These factors include effects of the blending agent on Reid vapor pressure, octane rating and oxygen content of the fuel. Blending incentives which account for these factors have been calculated by various sources. Unfortunately, they are based on old data and do not include a product similar in composition to the proposed mixed alcohol. Thus a model must be developed or acquired to recalculate these blending incentives blending before the actual competitiveness of the mixed alcohol in this capacity can be determined.

A preliminary environmental analysis indicates that BACT (Best Available Control Technology) will be required for construction of a coal to syngas to higher alcohols process due to the presence of H_2S and ozones above the threshold limits. This could have a significant effect on the cost of construction and operation of the process.

While the mixed alcohol product appears to be at least marginally competitive as a fuel additive, this is not necessarily the case for its usefulness as neat fuel. Although a plant gate cost in the range of $0.65-$0.66/gal. depending on the technology employed is less than the current refinery price of gasoline at $0.76/gal excluding taxes, the mixed alcohol is still more expensive due to its lower heat content (see Figures 2.5 and 2.6). This can be attributed to the fact that the mixed alcohol product is comprised of mainly methanol and ethanol with only small amounts of higher alcohols. Given the composition of the mixed alcohol, its price in relative terms based on its heat

Gasoline Consumption for West Virginia and Neighboring States

	WV	PA	MD	NJ	DC	DE	OH	KY	Total Local Market	Total U.S.	a	b
MM gal/yr	820	4488	1980	3272	169	335	4614	1797	17474	110922	170	1336
MM bbl/yr	19.5	106.8	47.1	77.9	4.0	8.0	109.9	42.8	416.0	2641.0	4.0	32

Local Market Potential for Mixed Alcohol as a Fuel Oxygenant (10 % Blend)

	WV	PA	MD	NJ	DC	DE	OH	KY	Total Local Market	Total U.S.
MM gal/yr	82	449	198	327	17	33	461	180	1747	11092
MM bbl/yr	2.0	10.7	4.7	7.8	0.4	0.8	11.0	4.3	41.6	264.1

a - Proposed Alcohol Production from Base Case Rev. 3 8/19/92:
b - Proposed Alcohol Production from Base Case Scale-Up:

Consumption Figures Are For 1990

Source : State Energy Data Report Consumption Est. 1960-1990 EIA May 1992.

Table 2.8

COAL DERIVED ALCOHOL FUEL

Gate Cost as a Function of Capacity

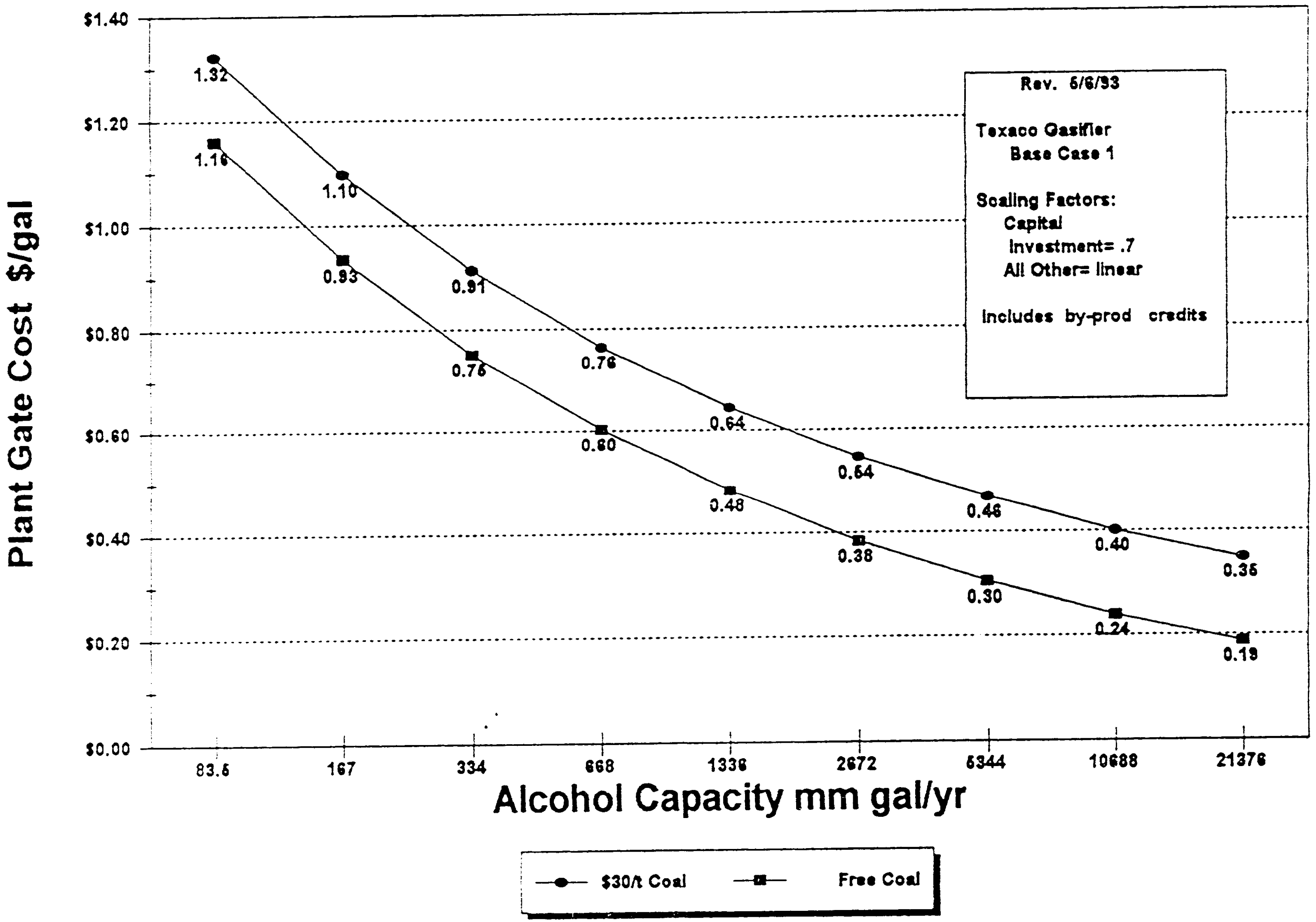


Figure 2.5

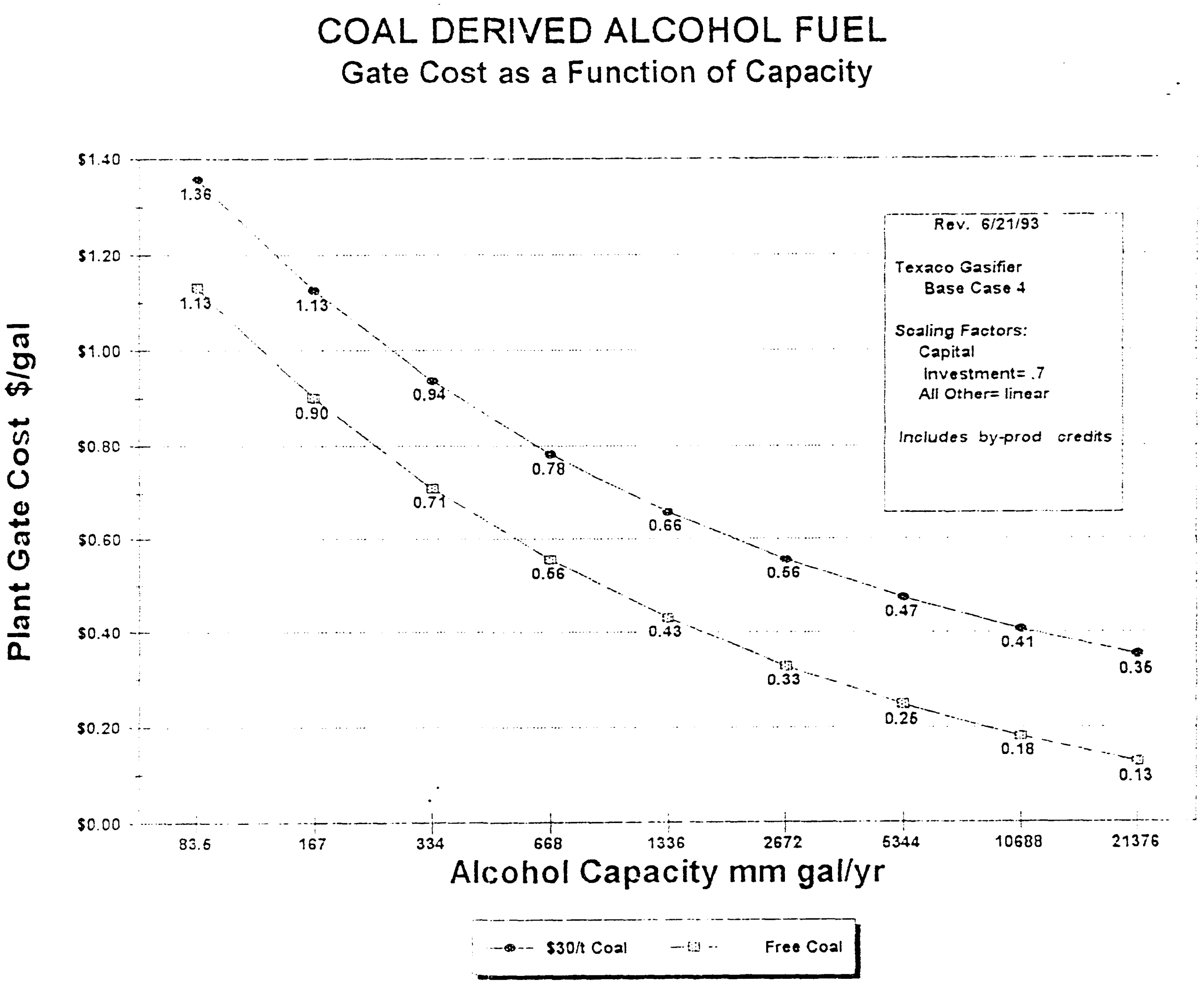

COAL DERIVED ALCOHOL FUEL
Gate Cost as a Function of Capacity
Plant Gate Cost $/gal
$1.40
$1.20
$1.00
$0.80
$0.60
$0.40
$0.20
$0.00
Alcohol Capacity mm gal/yr
83.6
167
334
668
1336
2672
5344
10688
21376
1.36
1.13
0.94
0.78
0.66
0.56
0.47
0.41
0.36
1.13
0.90
0.71
0.56
0.43
0.33
0.25
0.18
0.13
Rev. 6/21/93
Texaco Gasifier
Base Case 4
Scaling Factors:
Capital
Investment= .7
All Other= linear
Includes by-prod credits
$30/t Coal
Free Coal

Figure 2.6

content would be about $1.07/gal. which is substantially more than gasoline considering that this is a plant gate or break-even cost. The high concentration of methanol in this mixture may also present a series of problems that would be avoided by dilution if used as an additive. These problems are discussed in detail in the Fourth Quarter report for 1992.

The small concentrations of organic acids formed as a result of the hydrolysis of the esters (methyl acetate and ethyl acetate) will contribute negligibly to corrosion of the fuel storage and combustion systems. Hence, it may not be necessary to remove the esters from the alcohol mix. Presence of Cl^- ions, even in the concentration range of 10 ppm, should be avoided in the alcohol blend. Very small quantities of Cl^- causes severe corrosion. Discussions with the additive industry has revealed that effective corrosion inhibitors for gasoline-alcohol blends are not available in the market. As per the information available to date, the gasoline-alcohol blends should not contain more than 3.7% weight oxygen. The "substantially similar" clause imposed by the EPA will have to be met before the fuels produced by this group could be used on a commercial basis.

2.4 Recommendations

The amount of methanol in the mixed alcohol product should be reduced if possible to avoid potential problems. It appears that the level of methanol is a limiting factor in all current EPA waivers for fuel oxygenates. Given the current composition of the mixed alcohol, the amount of this alcohol that could be added to gasoline would be ten percent by volume due to its high concentration of methanol. The addition of larger volume would require the acquisition of a new waiver. This could be a costly and time consuming process. On the other hand, if the alcohol is to be used as a neat fuel in current engines, corrosion problems will inevitably need to be addressed if the methanol concentration is not reduced.

2.5 Future Plans

Base Cases 5 and 6, involving Shell gasification and either natural gas or a sour gas shift converter will be completed soon. Then the economics of scale-up will be investigated. As soon as the optimization methodology is developed for the alcohol synthesis section of the process, it will be applied to the entire process.

The current economic evaluation of scale-up, although general in nature, provides some direction with regard to the courses of action needed. However, refinement in these areas are essential to the overall advancement of the project. Therefore, joint efforts will be undertaken to refine the scale up of the current base cases and to develop the use incentives required to evaluate the actual competitiveness of the mixed alcohol.

With a clearer understanding of what is expected of the fuels produced by this group, the Fuels Evaluation group will blend n-butanol, propanol, ethanol and methanol with the ultimate goal of maintaining the oxygen level below 3.7% by weight keeping methanol content as low as possible. The next quarter will be devoted to blending the fuels, analyzing the physical and chemical properties of these blends and running engine tests with these blends for performance and emissions evaluations.

2.6 Appendix 1 for Task 2

Appendix 1 contains the environmental analysis of the sulfur removal portion of Base Case 1.

2.7 References for Task 2

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EMISSIONS FROM THE SULFUR REMOVAL PROCESS
BASE CASE 1

Base Case 1 is primarily a model of a process that will turn coal into an alcohol based fuel additive. This plant is very large, and will have a production of roughly 0.5 million metric tons of mixed alcohols per year. In order to properly design this Plant, it is important to compare the emissions of this facility with the Threshold Emission levels allowed by the government before Best Available Control Technology (BACT) is required. If BACT is required it will significantly affect the cost of our plant. The emissions were estimated from the Sulfur Removal portion of the plant because all of the sulfur compounds, along with a major part of the plant's CO, ozone producing compounds (VOC's that are precursors to ozone formation), and two Hazardous Air Pollutants (HAP's), methanol and COS, are found in this part of the process. After the estimations were completed, it was found that the H_2S, Total Reduced Sulfur (including H_2S), Reduced Sulfur Compounds (including H_2S and COS), Ozone producing VOC's, and the HAP's were all above the Threshold Values.

If the size of the plant increases, the total emissions will also increase. The stack emissions will go up with any raise in production. However, the fugitive emissions will grow only if the amount of equipment increases, for example, more trains are added.

The estimation of emissions for the sulfur removal process, which includes four blocks from Base Case 1 ; the Rectisol, COS Hydrolysis, Claus, and Beavon blocks (see Figure A.1), includes stack emissions and an estimation of the fugitive emissions for the blocks. The stack emissions were taken from the Base Case 1 flowsheet (see Figure A.1 and Tables A.47), while the fugitive emissions had to be estimated.

The fugitive emissions were estimated by using average emission factors.

$$E_{ij} = m_j F_i N_i$$

i = a type of equipment
j = a component
E_{ij} = Emissions of component j in equip. i (kg/hr)
m_j = mass fraction of component i
F_i = SOCMI Emission Factor for equipment i (kg/hr/source)
N_i = number of equipment i

The average emission factors (F_i) were taken from the Average Emission Factors for Synthetic Organic Chemical Manufacturing Industry (SOCMI) Fugitive Emissions (see Table A.1), which was taken from the U.S. Environmental Protection Agency, Emission Factors for Equipment Leaks of VOC and HAP, EPA-450/3-86-002, Research Triangle Park, NC, 1986.

Table A.1

EQUIPMENT	SERVICE	EMISSIONS FACTOR, kg/hr/source
Valves	Gas	0.0056
	Light Liquid	0.0071
	Heavy Liquid	0.00023
Pumps	Light Liquid	0.0494
	Heavy Liquid	0.0214
Compressors	Gas	0.228
Pressure Relief Valves	Gas	0.104
Flanges and Other Connectors	All	0.00083
Open-Ended Lines	All	0.0017
Sampling Connectors	All	0.015

A "light liquid " is defined by SOCMI as any fluid that is a liquid at the operating conditions and that either:

(1) Has a vapor pressure greater than 0.3 kPa at 20°C, or

(2) Contains at least 20% (by weight) of any component that has a vapor pressure greater than 0.3 kPa at 20°C.

A "heavy liquid" is any fluid that is a liquid at the operating conditions and that is not a "light liquid."

The mass fractions for each component in every stream were estimated from actual flowsheets and process specifications. The last estimation made was the quantity of each type of equipment that released fugitive emissions. This estimation involved a classification of each piece of equipment. For example, a reactor would be classified as a vertical vessel (see Table A.2). From these classifications, the total number of valves could be calculated, by using the Valve Estimations provided by the Chemical

Manufacturers Association, Improving Air Quality: Guidance for Estimating Fugitive Emissions from Equipment, p. 25, Washington, DC, January 1989, along with a correlation of the quantity of valves to the number of open-ended lines and flanges.

Table A.2

VALVE ESTIMATION	
Flow Sheet Predicting Item	Estimating Factor Valves per Item
Pressure Relief Valves	3
Flow Transmitter	6
Storage	13
Pump	11
Turbine Meter and Prover Connection	14
Vertical Vessel (reactor)	23
Horizontal Vessel (settler)	21
Heat Exchanger-Heated Side	8
Heat Exchanger-Cooled Side	17
Loading or Unloading Point	4

Number of open ended lines = 50% of the number of valves

Number of flanges = 420% of the number of valves

After the estimations and calculations were completed, the total emissions for the sulfur removal process were compared to the West Virginia Administrative Regulations, Air Pollution Control Commission, Chapter 16-20, Series 14, p. 14-5, 1984. If the quantity of a substance released is above its threshold value, then BACT applies. Table A.3 shows the comparison.

Table A.3

SIGNIFICANT EMISSIONS FROM THE SULFUR REMOVAL PROCESS

CLASSIFICATION	COMPONENTS EMITTED	THRESHOLD VALUES (ton/yr)	TOTAL EMISSIONS (ton/yr)
CO	CO	100	42.13
NOx	n/a	40	0
SOx	SO2	40	2.44
H2S	H2S	10	19.06
Total Reduced Sulfur Including H2S	H2S	10	19.06
Reduced Sulfur Compounds Including H2S	H2S, COS	10	19.76
Ozone (VOC excluding non-reactives)	CH3OH	40	4571.6

The total emissions for the sulfur removal process were compared to the 1990 Clean Air Act Amendment, Section 301. Any plant that emits 25 tons per year of any combination of HAP's, or more than 10 tons per year of any HAP compound is classified as a "major source" and is subject to stringent air pollution control. This portion of the plant has two HAP's: methanol and COS. The COS emitted is 0.71 tons per year, which is well below the limit. However, the methanol is well above the limit, 4571.6 tons per year, which pushes the plant over the combined 25 tons per year limit by 4547.3 tons per year. Thus, the plant is a major source of HAP's.

The conclusion is that for SO_x compounds, we will have no trouble meeting regulations because no other place in our plant has any SO_x. However, H_2S, Total Reduced Sulfur Including H_2S, Reduced Sulfur Compounds Including H_2S, and Ozone (VOC excluding non-reactives) are above the thresholds for BACT. The threshold value is not just for a particular part of the plant, it is a cumulative valve that includes the entire plant. Therefore it is a possibility that CO emissions will surpass the threshold, along with an increase in the Ozone (VOC) emissions because all of the alcohols (which are VOC's) are produced in the other portion of the plant. Also the plant is well over the HAP's limit, due to the huge amount of methanol going up the stack.

The following tables (A.4-A.6) contain a summary of the emissions from the Stack, the fugitive emissions, and the total emissions for the sulfur removal process.

Table A.4

STACK EMISSIONS FROM THE SULFUR REMOVAL PROCESS

COMPONENT	STACK EMISSIONS FROM: Rectisol Plant (kgmol/hr)	Beavon Plant (kgmol/hr)	TOTAL STACK EMISSIONS (kgmol/hr)	TOTAL STACK EMISSIONS (ton/yr)
CO2	1535	84.2	1619.2	560983
N2	2782.5	142.1	2924.6	644794
CH3OH	0	18	18	4535
NH3	0	8.3	8.3	1111

Table A.5

ESTIMATED FUGITIVE EMISSIONS FROM THE SULFUR REMOVAL PROCESS

COMPONENT	SULFUR REMOVAL EMISSIONS FROM: Rectisol (kg/hr)	COS Hydrolysis (kg/hr)	Claus (kg/hr)	Beavon (kg/hr)	TOTAL SULFUR REMOVAL EMISSIONS (ton/yr)
CH3OH	3.91	0.11	0.38	0.25	36.61
CH4	0.02	0	0	0	0.16
CO	4.06	1.29	0	0	42.13
CO2	4.16	0.71	2.47	1.63	70.63
COS	0.05	0.04	0	0	0.71
H2	0.37	0	0	0	2.91
H2O	1.25	0	0.49	4.55	49.53
H2S	0.57	0.49	0.78	0.58	19.06
N2	0.65	0.08	2.06	3.08	46.22
NH3	0.01	0.03	0.09	0.06	1.50
O2	0	0.02	0.15	0.18	2.76
SO2	0	0	0.31	0	2.44

Table A.6

TOTAL (stack plus fugitive) EMISSIONS FROM THE SULFUR REMOVAL PROCESS

CLASSIFICATION	COMPONENTS EMITTED	THRESHOLD VALUES (ton/yr)	TOTAL EMISSIONS (ton/yr)
CO	CO	100	42.13
NOx	n/a	40	0
SOx	SO2	40	2.44
H2S	H2S	10	19.06
Total Reduced Sulfur Including H2S	H2S	10	19.06
Reduced Sulfur Compounds Including H2S	H2S, COS	10	19.76
Ozone (VOC excluding non-reactives)	CH3OH	40	4571.6

RECTISOL PLANT

The flowsheet for the Rectisol Plant was taken from the Houston Area Medium-BTU Coal Gasification Project Final Report, published in June 1982 by Union Carbide (Further references to this will be referred to as Houston). The information needed for the flow estimations was taken from Houston as well as the Gas Process Handbook '92, Hydrocarbon Processing, April 1992, p. 125.

Table A.7

RECTISOL PLANT OVERALL FUGITIVE EMISSIONS
FOR TWO TRAINS

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open-Ended Lines (kg/hr)	
CO	2.02E+00	0	4.22E-01	1.76E-01	1.16E+00	2.83E-01	4.06
CO2	2.25E+00	0	0	4.14E-01	1.20E+00	2.93E-01	4.16
COS	2.75E-02	1.45E-03	0	1.51E-03	1.39E-02	3.39E-03	0.05
H2	1.89E-01	0	3.42E-02	1.42E-02	1.06E-01	2.59E-02	0.37
H2O	6.64E-01	0	0	1.43E-01	3.57E-01	8.71E-02	1.25
H2S	3.30E-01	1.98E-02	0	1.41E-02	1.65E-01	4.03E-02	0.57
N2	3.64E-01	0	0	7.42E-03	2.23E-01	5.44E-02	0.65
NH3	7.83E-03	0	0	8.27E-04	4.04E-03	9.85E-04	0.01
CH4	1.30E-02	0	0	2.47E-03	6.95E-03	1.69E-03	0.02
CH3OH	2.21E+00	2.75E-01	0	5.92E-02	1.10E+00	2.69E-01	3.91

The following tables (A.8-A.23) are the actual estimations made for the Rectisol Plant in Base Case 1.

Table A.8

ESTIMATION OF FUGITIVE EMISSIONS FOR THE RECTISOL PLANT

RECTISOL PLANT	
QUANTITY	EQUIPMENT TYPE
3	Pumps
7	Vertical Vessles
0	Horizontal Vessles
0	Storage Tanks
4	Pressure Relief Valves
3	Heat - Exchangers (Heating Side)
6	Heat - Exchangers (Cooling Side)
0	Loading or Unloading Point
37	Flow Transmitters
0	Turbine Meter and Prover Connection

QUANTITY	ACTUAL EQUIPMENT
3	Separators (Knockout Drums)
4	Towers
4	Heat Exchangers
3	Pumps
1	Compressor
4	Pressure Relief Valves
37	Flow Transmitters

QUANTITY	ESTIMATED EQUIPMENT
623	Valves
312	Open - Ended Lines
2617	Flanges

QUANTITY	EQUIPMENT WITH FUGITIVES
623	Valves
3	Pumps
1	Compressors
4	Pressure Relief Valves
2617	Flanges
312	Open - Ended Lines

Table A.9

INLET STREAM (gas)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE UNSHIFTED RECTISOL TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	0
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	2
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	4673	130830	4.55E-01
CO2	1616	71113	2.47E-01
COS	4	210	7.30E-04
H2	5260	10520	3.66E-02
H2O	3900	70193	2.44E-01
H2S	72	2448	8.51E-03
N2	46	1277	4.44E-03
NH3	8	141	4.90E-04
CH4	27	426	1.48E-03
CH3OH	18	576	2.00E-03
TOTAL FLOW	15622	287733	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0	0.00083	0.0017
QUANTITY	12	0	0	0	50	6

COMPONENT	EMISSIONS FROM:						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	3.06E-02	0	0	0	1.90E-02	4.64E-03	5.42E-02
CO2	1.66E-02	0	0	0	1.03E-02	2.52E-03	2.95E-02
COS	4.90E-05	0	0	0	3.05E-05	7.44E-06	8.70E-05
H2	2.46E-03	0	0	0	1.53E-03	3.73E-04	4.36E-03
H2O	1.64E-02	0	0	0	1.02E-02	2.49E-03	2.91E-02
H2S	5.72E-04	0	0	0	3.56E-04	8.68E-05	1.01E-03
N2	2.98E-04	0	0	0	1.86E-04	4.53E-05	6.29E-04
NH3	3.30E-05	0	0	0	2.05E-05	5.00E-06	5.85E-05
CH4	9.94E-05	0	0	0	6.19E-05	1.51E-05	1.76E-04
CH3OH	1.35E-04	0	0	0	8.37E-05	2.04E-05	2.39E-04

Table A.10

FEED HEAT EXCHANGER AND KNOCKOUT VESSEL (gas)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE UNSHIFTED RECTISOL TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	1
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	1
Loading or Unloading Point	0
Flow Transmitters	2
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	3037	85037	5.15E-01
CO2	808	35556	2.15E-01
COS	2	105	6.36E-04
H2	3425	6850	4.15E-02
H20	1950	35096	2.13E-01
H2S	36	1224	7.41E-03
N2	23	638	3.87E-03
NH3	4	71	4.27E-04
CH4	13	213	1.29E-03
CH3OH	9	288	1.74E-03
TOTAL FLOW	9307	165079	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0	0.00083	0.0017
QUANTITY	52	0	0	0	218	26

COMPONENT	EMISSIONS (kg/hr) FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	1.50E-01	0	0	0	9.34E-02	2.28E-02	2.66E-01
CO2	6.27E-02	0	0	0	3.90E-02	9.52E-03	1.11E-01
COS	1.85E-04	0	0	0	1.15E-04	2.81E-05	3.29E-04
H2	1.21E-02	0	0	0	7.52E-03	1.83E-03	2.14E-02
H20	6.19E-02	0	0	0	3.85E-02	9.40E-03	1.10E-01
H2S	2.16E-03	0	0	0	1.34E-03	3.28E-04	3.83E-03
N2	1.13E-03	0	0	0	7.01E-04	1.71E-04	2.00E-03
NH3	1.24E-04	0	0	0	7.75E-05	1.89E-05	2.21E-04
CH4	3.75E-04	0	0	0	2.34E-04	5.70E-05	6.66E-04
CH3OH	5.08E-04	0	0	0	3.16E-04	7.71E-05	9.01E-04

Table A.11

GAS ABSORBER WASH TOWER (gas)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE UNSHIFTED RECTISOL TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	1
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	1
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	4673	130830	4.55E-01
CO2	1616	71113	2.47E-01
COS	4	210	7.30E-04
H2	5260	10520	3.66E-02
H20	3900	70193	2.44E-01
H2S	72	2448	8.51E-03
N2	46	1277	4.44E-03
NH3	8	141	4.90E-04
CH4	27	426	1.48E-03
CH3OH	18	576	2.00E-03
TOTAL FLOW	15622	287733	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0	0.00083	0.0017
QUANTITY	29	0	0	0	122	15

COMPONENT	EMISSIONS (kg/hr) FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	7.38E-02	0	0	0	4.60E-02	1.12E-02	1.31E-01
CO2	4.01E-02	0	0	0	2.50E-02	8.09E-03	7.12E-02
COS	1.19E-04	0	0	0	7.38E-05	1.80E-05	2.10E-04
H2	5.94E-03	0	0	0	3.70E-03	9.01E-04	1.05E-02
H20	3.96E-02	0	0	0	2.47E-02	6.01E-03	7.03E-02
H2S	1.38E-03	0	0	0	8.60E-04	2.10E-04	2.45E-03
N2	7.21E-04	0	0	0	4.49E-04	1.09E-04	1.28E-03
NH3	7.96E-05	0	0	0	4.96E-05	1.21E-05	1.41E-04
CH4	2.40E-04	0	0	0	1.50E-04	3.65E-05	4.26E-04
CH3OH	3.25E-04	0	0	0	2.02E-04	4.93E-05	5.77E-04

Table A.12

GAS ABSORBER WASH TOWER (liquid)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE UNSHIFTED RECTISOL TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	1
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	1
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	0	0	0
CO2	0	0	0
COS	0	0	0
H2	0	0	0
H20	0	0	0
H2S	0	0	0
N2	0	0	0
NH3	0	0	0
CH4	0	0	0
CH3OH	100	3200	1
TOTAL FLOW	100	3200	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0071	0	0	0	0.00083	0.0017
QUANTITY	29	0	0	0	122	15

COMPONENT	EMISSIONS (kg/hr) FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	0	0	0	0	0	0	0
CO2	0	0	0	0	0	0	0
COS	0	0	0	0	0	0	0
H2	0	0	0	0	0	0	0
H2O	0	0	0	0	0	0	0
H2S	0	0	0	0	0	0	0
N2	0	0	0	0	0	0	0
NH3	0	0	0	0	0	0	0
CH4	0	0	0	0	0	0	0
CH3OH	0.21	0	0	0	0.10	0.02	3.32E-01

Table A.13

H2, CO RECLAIMER #1 (liquid)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE UNSHIFTED RECTISOL TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	1
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	1
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	1
Loading or Unloading Point	0
Flow Transmitters	3
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	350	9811	4.31E-01
CO2	269	11854	5.21E-01
COS	0	0	0.00E+00
H2	395	789	3.47E-02
H2O	0	0	0.00E+00
H2S	0	0	0.00E+00
N2	8	213	9.35E-03
NH3	1	23	1.03E-03
CH4	4	71	3.11E-03
CH3OH	0	0	0.00E+00
TOTAL FLOW	1028	22761	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0071	0	0	0.104	0.00083	0.0017
QUANTITY	61	0	0	1	256	31

COMPONENT	EMISSIONS (kg/hr) FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	1.87E-01	0	0	4.48E-02	9.17E-02	2.24E-02	3.46E-01
CO2	2.26E-01	0	0	5.42E-02	1.11E-01	2.70E-02	4.17E-01
COS	0	0	0	0	0	0	0
H2	1.50E-02	0	0	3.61E-03	7.37E-03	1.80E-03	2.78E-02
H2O	0	0	0	0	0	0	0
H2S	0	0	0	0	0	0	0
N2	4.05E-03	0	0	9.72E-04	1.99E-03	4.85E-04	7.49E-03
NH3	4.46E-04	0	0	1.07E-04	2.19E-04	5.34E-05	8.26E-04
CH4	1.35E-03	0	0	3.24E-04	6.62E-04	1.61E-04	2.50E-03
CH3OH	0	0	0	0	0	0	0

Table A.14

H2, CO RECLAIMER #2 (liquid)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE UNSHIFTED RECTISOL TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	1
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	1
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	1
Loading or Unloading Point	0
Flow Transmitters	3
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	350	9811	4.15E-01
CO2	269	11854	5.01E-01
COS	1	70	2.97E-03
H2	395	789	3.34E-02
H20	0	0	0
H2S	24	816	3.45E-02
N2	8	213	9.00E-03
NH3	1	23	9.92E-04
CH4	4	71	3.00E-03
CH3OH	0	0	0
TOTAL FLOW	1053	23647	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0071	0	0	0.104	0.00083	0.0017
QUANTITY	61	0	0	1	256	31

COMPONENT	EMISSIONS (kg/hr) FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	1.80E-01	0	0	4.31E-02	8.82E-02	2.15E-02	3.33E-01
CO2	2.17E-01	0	0	5.21E-02	1.07E-01	2.60E-02	4.02E-01
COS	1.29E-03	0	0	3.09E-04	6.31E-04	1.54E-04	2.38E-03
H2	1.45E-02	0	0	3.47E-03	7.10E-03	1.73E-03	2.87E-02
H20	0	0	0	0	0	0	0
H2S	1.49E-02	0	0	3.59E-03	7.34E-03	1.79E-03	2.77E-02
N2	3.90E-03	0	0	9.36E-04	1.91E-03	4.67E-04	7.21E-03
NH3	4.30E-04	0	0	1.03E-04	2.11E-04	5.14E-05	7.95E-04
CH4	1.30E-03	0	0	3.12E-04	6.37E-04	1.55E-04	2.40E-03
CH3OH	0	0	0	0	0	0	0

Table A.15

H2, CO RECYCLE STREAM (gas)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE UNSHIFTED RECTISOL TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	0
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	1
Loading or Unloading Point	0
Flow Transmitters	5
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	701	19622	9.25E-01
CO2	0	0	0
COS	0	0	0
H2	795	1590	7.50E-02
H20	0	0	0
H2S	0	0	0
N2	0	0	0
NH3	0	0	0
CH4	0	0	0
CH3OH	0	0	0
TOTAL FLOW	1496	21212	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0.228	0	0.00083	0.0017
QUANTITY	47	0	1	0	197	24

COMPONENT	EMISSIONS (kg/hr) FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	2.43E-01	0	2.11E-01	0	1.52E-01	3.70E-02	6.43E-01
CO2	0	0	0	0	0	0	0
COS	0	0	0	0	0	0	0
H2	1.97E-02	0	1.71E-02	0	1.23E-02	2.99E-03	5.21E-02
H20	0	0	0	0	0	0	0
H2S	0	0	0	0	0	0	0
N2	0	0	0	0	0	0	0
NH3	0	0	0	0	0	0	0
CH4	0	0	0	0	0	0	0
CH3OH	0	0	0	0	0	0	0

Table A.16

PURIFIED GAS STREAM
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE UNSHIFTED RECTISOL TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	0
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	2
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	2
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	2336	65415	9.26E-01
CO2	0	0	0
COS	0	0	0
H2	2630	5260	7.44E-02
H2O	0	0	0
H2S	0	0	0
N2	0	0	0
NH3	0	0	0
CH4	0	0	0
CH3OH	0	0	0
TOTAL FLOW	4966	70675	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0	0.00083	0.0017
QUANTITY	28	0	0	0	118	14

COMPONENT	EMISSIONS (kg/hr) FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	1.45E-01	0	0	0	9.03E-02	2.20E-02	2.58E-01
CO2	0	0	0	0	0	0	0
COS	0	0	0	0	0	0	0
H2	1.17E-02	0	0	0	7.26E-03	1.77E-03	2.07E-02
H2O	0	0	0	0	0	0	0
H2S	0	0	0	0	0	0	0
N2	0	0	0	0	0	0	0
NH3	0	0	0	0	0	0	0
CH4	0	0	0	0	0	0	0
CH3OH	0	0	0	0	0	0	0

Table A.17

UNSHIFTED GAS METHANOL - WATER SEPARATION TOWER (liquid)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE UNSHIFTED RECTISOL TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	1
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	1
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	3
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	0	0	0
CO2	539	23716	2.32E-01
COS	1	60	5.86E-04
H2	0	0	0
H20	3900	70200	6.86E-01
H2S	24	816	7.97E-03
N2	15	420	4.10E-03
NH3	3	51	4.98E-04
CH4	9	144	1.41E-03
CH3OH	218	6976	6.81E-02
TOTAL FLOW	4709	102383	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0071	0	0	0.104	0.00083	0.0017
QUANTITY	44	0	0	1	185	22

COMPONENT	EMISSIONS (kg/hr) FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	0	0	0	0	0	0	0
CO2	7.24E-02	0	0	2.41E-02	3.55E-02	8.66E-03	1.41E-01
COS	1.83E-04	0	0	6.09E-05	8.99E-05	2.19E-05	3.56E-04
H2	0	0	0	0	0	0	0
H20	2.14E-01	0	0	7.13E-02	1.05E-01	2.56E-02	4.16E-01
H2S	2.49E-03	0	0	8.29E-04	1.22E-03	2.98E-04	4.84E-03
N2	1.28E-03	0	0	4.27E-04	6.29E-04	1.53E-04	2.49E-03
NH3	1.56E-04	0	0	5.18E-05	7.64E-05	1.86E-05	3.02E-04
CH4	4.39E-04	0	0	1.46E-04	2.16E-04	5.26E-05	8.54E-04
CH3OH	2.13E-02	0	0	7.09E-03	1.05E-02	2.55E-03	4.14E-02

Table A.18

UNSHIFTED GAS STRIPPING COLUMN (liquid)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE UNSHIFTED RECTISOL TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	1
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	2
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	0	0	0
CO2	539	23716	7.91E-01
COS	1	60	2.00E-03
H2	790	1580	5.27E-02
H2O	0	0	0
H2S	24	816	2.72E-02
N2	15	420	1.40E-02
NH3	3	51	1.70E-03
CH4	9	144	4.80E-03
CH3OH	100	3200	1.07E-01
TOTAL FLOW	1481	29987	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0071	0	0	0	0.00083	0.0017
QUANTITY	35	0	0	0	147	18

COMPONENT	EMISSIONS (kg/hr) FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	0	0	0	0	0	0	0
CO2	1.97E-01	0	0	0	9.65E-02	2.35E-02	3.17E-01
COS	4.97E-04	0	0	0	2.44E-04	5.95E-05	8.01E-04
H2	1.31E-02	0	0	0	6.43E-03	1.57E-03	2.11E-02
H2O	0	0	0	0	0	0	0
H2S	6.76E-03	0	0	0	3.32E-03	8.10E-04	1.09E-02
N2	3.48E-03	0	0	0	1.71E-03	4.17E-04	5.61E-03
NH3	4.23E-04	0	0	0	2.08E-04	5.06E-05	6.81E-04
CH4	1.19E-03	0	0	0	5.86E-04	1.43E-04	1.92E-03
CH3OH	2.65E-02	0	0	0	1.30E-02	3.17E-03	4.27E-02

Table A.19

UNSHIFTED GAS STRIPPING COLUMN (gas)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE UNSHIFTED RECTISOL TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	1
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	1
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	0	0	0
CO2	0	0	0
COS	0	0	0
H2	0	0	0
H20	0	0	0
H2S	0	0	0
N2	1368	38304	1
NH3	0	0	0
CH4	0	0	0
CH3OH	0	0	0
TOTAL FLOW	1368	38304	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0	0.00083	0.0017
QUANTITY	29	0	0	0	122	15

COMPONENT	EMISSIONS (kg/hr) FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	0	0	0	0	0	0	0
CO2	0	0	0	0	0	0	0
COS	0	0	0	0	0	0	0
H2	0	0	0	0	0	0	0
H20	0	0	0	0	0	0	0
H2S	0	0	0	0	0	0	0
N2	1.62E-01	0	0	0	1.01E-01	2.47E-02	2.88E-01
NH3	0	0	0	0	0	0	0
CH4	0	0	0	0	0	0	0
CH3OH	0	0	0	0	0	0	0

Table A.20

UNSHIFTED METHANOL REGENERATION TOWER (gas feed)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE UNSHIFTED RECTISOL TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	1
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	1
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	1
Loading or Unloading Point	0
Flow Transmitters	3
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	0	0	0
CO2	269	11854	7.36E-01
COS	1	60	3.72E-03
H2	0	0	0
H2O	0	0	0
H2S	12	408	2.53E-02
N2	8	213	1.32E-02
NH3	1	23	1.46E-03
CH4	4	70	4.37E-03
CH3OH	109	3488	2.16E-01
TOTAL FLOW	405	16116	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0.104	0.00083	0.0017
QUANTITY	61	0	0	1	256	31

COMPONENT	EMISSIONS (kg/hr) FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	0	0	0	0	0	0	0
CO2	2.51E-01	0	0	7.65E-02	1.56E-01	3.81E-02	5.22E-01
COS	1.27E-03	0	0	3.87E-04	7.92E-04	1.93E-04	2.64E-03
H2	0	0	0	0	0	0	0
H2O	0	0	0	0	0	0	0
H2S	8.65E-03	0	0	2.63E-03	5.38E-03	1.31E-03	1.80E-02
N2	4.51E-03	0	0	1.37E-03	2.81E-03	6.85E-04	9.38E-03
NH3	4.97E-04	0	0	1.51E-04	3.10E-04	7.55E-05	1.03E-03
CH4	1.49E-03	0	0	4.54E-04	9.29E-04	2.26E-04	3.10E-03
CH3OH	7.39E-02	0	0	2.25E-02	4.60E-02	1.12E-02	1.54E-01

Table A.21

UNSHIFTED METHANOL REGENERATION TOWER (liquid feed)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE UNSHIFTED RECTISOL TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	1
Vertical Vessles	1
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	1
Loading or Unloading Point	0
Flow Transmitters	3
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	0	0	0
CO2	0	0	0
COS	1	60	1.47E-02
H2	0	0	0
H20	0	0	0
H2S	24	816	2.00E-01
N2	0	0	0
NH3	0	0	0
CH4	0	0	0
CH3OH	100	3200	7.85E-01
TOTAL FLOW	125	4076	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0071	0.0494	0	0	0.00083	0.0017
QUANTITY	69	1	0	0	290	35

COMPONENT	EMISSIONS (kg/hr) FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	0	0	0	0	0	0	0
CO2	0	0	0	0	0	0	0
COS	7.21E-03	7.27E-04	0	0	3.54E-03	8.63E-04	1.23E-02
H2	0	0	0	0	0	0	0
H20	0	0	0	0	0	0	0
H2S	9.81E-02	9.89E-03	0	0	4.82E-02	1.17E-02	1.68E-01
N2	0	0	0	0	0	0	0
NH3	0	0	0	0	0	0	0
CH4	0	0	0	0	0	0	0
CH3OH	3.85E-01	3.88E-02	0	0	1.89E-01	4.60E-02	6.58E-01

Table A.22

METHANOL RECYCLE STREAM (liquid)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE UNSHIFTED RECTISOL TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	2
Vertical Vessles	0
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	1
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	4
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	0	0	0
CO2	0	0	0
COS	0	0	0
H2	0	0	0
H2O	0	0	0
H2S	0	0	0
N2	0	0	0
NH3	0	0	0
CH4	0	0	0
CH3OH	200	6400	1
TOTAL FLOW	200	6400	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0071	0.0494	0	0	0.00083	0.0017
QUANTITY	54	2	0	0	227	27

COMPONENT	EMISSIONS (kg/hr) FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	0	0	0	0	0	0	0
CO2	0	0	0	0	0	0	0
COS	0	0	0	0	0	0	0
H2	0	0	0	0	0	0	0
H2O	0	0	0	0	0	0	0
H2S	0	0	0	0	0	0	0
N2	0	0	0	0	0	0	0
NH3	0	0	0	0	0	0	0
CH4	0	0	0	0	0	0	0
CH3OH	3.83E-01	9.88E-02	0	0	1.88E-01	4.59E-02	7.18E-01

Table A.23

H2S , COS RICH STREAM (gas)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE UNSHIFTED RECTISOL TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	0
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	2
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	0	0	0
CO2	81	3551	5.10E-01
COS	4	240	3.45E-02
H2	0	0	0
H20	0	0	0
H2S	72	2448	3.52E-01
N2	0	0	0
NH3	8	141	2.03E-02
CH4	0	0	0
CH3OH	18	576	8.28E-02
TOTAL FLOW	183	6956	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0071	0	0	0	0.00083	0.0017
QUANTITY	12	0	0	0	50	6

COMPONENT	EMISSIONS (kg/hr) FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	0	0	0	0	0	0	0
CO2	4.35E-02	0	0	0	2.14E-02	5.21E-03	7.01E-02
COS	2.94E-03	0	0	0	1.44E-03	3.52E-04	4.73E-03
H2	0	0	0	0	0	0	0
H2O	0	0	0	0	0	0	0
H2S	3.00E-02	0	0	0	1.47E-02	3.59E-03	4.83E-02
N2	0	0	0	0	0	0	0
NH3	1.73E-03	0	0	0	8.49E-04	2.07E-04	2.78E-03
CH4	0	0	0	0	0	0	0
CH3OH	7.06E-03	0	0	0	3.46E-03	8.45E-04	1.14E-02

COS HYDROLYSIS PLANT

The flowsheet for the COS hydrolysis along with the information needed for the stream estimations were taken from the Gas Process Handbook '84, Hydrocarbon Processing, April 1984, p. 78.

Table A.24

COS HYDROLYSIS PLANT OVERALL FUGITIVE EMISSIONS

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressor (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open-Ended Lines (kg/hr)	
CO	6.27E-01	0	0	1.82E-01	3.90E-01	9.52E-02	1.29
CO2	3.42E-01	0	0	9.93E-02	2.13E-01	5.19E-02	0.71
COS	2.02E-02	0	0	5.87E-03	1.26E-02	3.07E-03	0.04
H2	6.75E-04	0	0	1.96E-04	4.20E-04	1.02E-04	0
H2S	2.36E-01	0	0	6.85E-02	1.47E-01	3.58E-02	0.49
N2	3.78E-02	0	0	1.10E-02	2.35E-02	5.73E-03	0.08
NH3	1.36E-02	0	0	3.95E-03	8.47E-03	2.06E-03	0.03
CH3OH	5.55E-02	0	0	1.61E-02	3.46E-02	8.43E-03	0.11
O2	1.08E-02	0	0	3.13E-03	6.72E-03	1.64E-03	0.02

The following tables (A.25-A.27) are the actual estimations made for the COS Hydrolysis Plant in Base Case 1.

Table A.25

ESTIMATION OF FUGITIVE EMISSIONS FOR THE COS HYDROLYSIS PLANT

COS HYDROLYSIS	
QUANTITY	EQUIPMENT TYPE
0	Pumps
1	Vertical Vessles
0	Horizontal Vessles
0	Storage Tanks
1	Pressure Relief Valves
1	Heat - Exchangers (Heating Side)
0	Heat - Exchangers (Cooling Side)
0	Loading or Unloading Point
5	Flow Transmitters
0	Turbine Meter and Prover Connection

QUANTITY	ACTUAL EQUIPMENT
1	Preheater
1	Hydrolysis Reactor
1	Pressure Relief Valves
5	Flow Transmitters

QUANTITY	ESTIMATED EQUIPMENT
64	Valves
32	Open - Ended Lines
269	Flanges

QUANTITY	EQUIPMENT WITH FUGITIVES
64	Valves
0	Pumps
0	Compressors
1	Pressure Relief Valves
269	Flanges
32	Open - Ended Lines

Table A.26

MIXER - PREHEATER
ESTIMATION OF FUGITIVE EMISSIONS FOR COS HYDROLYSIS

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	0
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	1
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	3
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	3.5	98	8.75E-01
CO2	81	3551	4.77E-01
COS	4	210	2.82E-02
H2	4	7	9.41E-04
H2S	72	2448	3.29E-01
N2	14	392	5.27E-02
NH3	8	141	1.90E-02
CH3OH	18	576	7.75E-02
O2	4	112	1.51E-02
TOTAL FLOW	204	7437	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0	0.00083	0.0017
QUANTITY	26	0	0	0	109	13

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	1.27E-01	0	0	0	7.93E-02	1.93E-02	2.26E-01
CO2	6.95E-02	0	0	0	4.33E-02	1.06E-02	1.23E-01
COS	4.11E-03	0	0	0	2.56E-03	6.24E-04	7.29E-03
H2	1.37E-04	0	0	0	8.53E-05	2.08E-05	2.43E-04
H2S	4.79E-02	0	0	0	2.98E-02	7.27E-03	8.50E-02
N2	7.67E-03	0	0	0	4.78E-03	1.16E-03	1.36E-02
NH3	2.76E-03	0	0	0	1.72E-03	4.19E-04	4.90E-03
CH3OH	1.13E-02	0	0	0	7.02E-03	1.71E-03	2.00E-02
O2	2.19E-03	0	0	0	1.36E-03	3.33E-04	3.89E-03

Table A.27

HYDROGENATION / HYDROLYSIS REACTOR
ESTIMATION OF FUGITIVE EMISSIONS FOR COS HYDROLYSIS

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	1
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	1
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	2
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO	0	0	0
CO2	84	3705	5.02E-01
COS	0	0	0
H2	0	0	0
H2S	76	2567	3.48E-01
N2	14	392	5.31E-02
NH3	8	141	1.91E-02
CH3OH	18	576	7.80E-02
O2	0	0	0
TOTAL FLOW	200	7381	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0.104	0.00083	0.0017
QUANTITY	38	0	0	1	160	19

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO	1.86E-01	0	0	9.10E-02	1.16E-01	2.83E-02	4.21E-01
CO2	1.02E-01	0	0	4.97E-02	6.32E-02	1.54E-02	2.30E-01
COS	6.01E-03	0	0	2.94E-03	3.74E-03	9.12E-04	1.36E-02
H2	2.00E-04	0	0	9.79E-05	1.25E-04	3.04E-05	4.53E-04
H2S	7.00E-02	0	0	3.42E-02	4.36E-02	1.06E-02	1.59E-01
N2	1.12E-02	0	0	5.48E-03	6.98E-03	1.70E-03	2.54E-02
NH3	4.04E-03	0	0	1.97E-03	2.51E-03	6.13E-04	9.14E-03
CH3OH	1.65E-02	0	0	8.05E-03	1.03E-02	2.50E-03	3.73E-02
O2	3.20E-03	0	0	1.57E-03	1.99E-03	4.86E-04	7.25E-03

CLAUS PLANT

The flowsheet for the Claus Plant was taken from Houston. The information needed for the flow estimations was taken from Houston as well as the Gas Process Handbook '84, Hydrocarbon Processing, April 1984, p. 74.

Table A.28

CLAUS PLANT OVERALL FUGITIVE EMISSIONS
FOR TWO TRAIN

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open-Ended Lines (kg/hr)	
CO2	1.24E+00	0	0	2.77E-01	7.71E-01	1.88E-01	2.47
H2O	2.40E-01	0	0	6.67E-02	1.50E-01	3.65E-02	0.49
H2S	4.04E-01	0	0	6.62E-02	2.51E-01	6.13E-02	0.78
N2	1.00E+00	0	0	2.87E-01	6.23E-01	1.52E-01	2.06
CH3OH	1.92E-01	0	0	4.61E-02	1.20E-01	2.92E-02	0.38
S	4.35E-02	0	0	8.06E-03	2.71E-02	6.60E-03	0.09
SO2	1.47E-01	0	0	5.19E-02	9.15E-02	2.23E-02	0.31
O2	7.01E-02	0	0	2.08E-02	4.36E-02	1.06E-02	0.15
NH3	4.71E-02	0	0	1.06E-02	2.93E-02	7.16E-03	0.09

The following tables (A.29-A.35) are the actual estimations made for the Claus Plant in Base Case 1.

Table A.29

ESTIMATION OF FUGITIVE EMISSIONS FOR THE CLAUS PLANT

<table>
<tr><th colspan="2">CLAUS PLANT</th></tr>
<tr><th>QUANTITY</th><th>EQUIPMENT TYPE</th></tr>
<tr><td>0</td><td>Pumps</td></tr>
<tr><td>6</td><td>Vertical Vessles</td></tr>
<tr><td>6</td><td>Horizontal Vessles</td></tr>
<tr><td>0</td><td>Storage Tanks</td></tr>
<tr><td>8</td><td>Pressure Relief Valves</td></tr>
<tr><td>8</td><td>Heat - Exchangers (Heating Side)</td></tr>
<tr><td>0</td><td>Heat - Exchangers (Cooling Side)</td></tr>
<tr><td>0</td><td>Loading or Unloading Point</td></tr>
<tr><td>28</td><td>Flow Transmitters</td></tr>
<tr><td>0</td><td>Turbine Meter and Prover Connection</td></tr>
</table>

QUANTITY	ACTUAL EQUIPMENT
2	Separators (Knockout Drums)
2	Thermal Incinerators
2	Boilers
6	Reheaters
2	3 - Staged Catalytic Reactors
2	Sulfur Condensers
8	Pressure Relief Valves
28	Flow Transmitters

QUANTITY	ESTIMATED EQUIPMENT
520	Valves
260	Open - Ended Lines
2184	Flanges

QUANTITY	EQUIPMENT WITH FUGITIVES
520	Valves
0	Pumps
0	Compressors
8	Pressure Relief Valves
2184	Flanges
260	Open - Ended Lines

Table A.30

SEPARATOR
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE CLAUS TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	0
Horizontal Vessles	1
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	5
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO2	84	3705	5.02E-01
H2O	0	0	0
H2S	76	2567	3.48E-01
N2	14	392	5.31E-02
CH3OH	18	576	7.80E-02
S	0	0	0
SO2	0	0	0
O2	0	0	0
NH3	8	141	1.91E-02
TOTAL FLOW	200	7381	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0	0.00083	0.0017
QUANTITY	51	0	0	0	214	26

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO2	1.43E-01	0	0	0	8.92E-02	2.18E-02	2.54E-01
H2O	0	0	0	0	0	0	0
H2S	9.93E-02	0	0	0	6.18E-02	1.51E-02	1.76E-01
N2	1.52E-02	0	0	0	9.44E-03	2.30E-03	2.69E-02
CH3OH	2.23E-02	0	0	0	1.39E-02	3.38E-03	3.95E-02
S	0	0	0	0	0	0	0
SO2	0	0	0	0	0	0	0
O2	0	0	0	0	0	0	0
NH3	5.46E-03	0	0	0	3.40E-03	8.29E-04	9.69E-03

Table A.31

THERMAL INCINERATOR AND BOILER
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE CLAUS TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	0
Horizontal Vessles	1
Storage Tanks	0
Pressure Relief Valves	1
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	1
Loading or Unloading Point	0
Flow Transmitters	0
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO2	28	1235	2.64E-01
H2O	15	262	5.61E-02
H2S	11	360	7.71E-02
N2	61	1699	3.64E-01
CH3OH	6	192	4.11E-02
S	6	181	3.88E-02
SO2	9	570	1.22E-01
O2	4	126	2.71E-02
NH3	3	47	1.01E-02
TOTAL FLOW	141	4673	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0.104	0.00083	0.0017
QUANTITY	41	0	0	1	172	21

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO2	6.07E-02	0	0	2.75E-02	3.78E-02	9.21E-03	1.35E-01
H2O	1.29E-02	0	0	5.84E-03	8.02E-03	1.96E-03	2.87E-02
H2S	1.77E-02	0	0	8.02E-03	1.10E-02	2.69E-03	3.94E-02
N2	8.35E-02	0	0	3.78E-02	5.20E-02	1.27E-02	1.86E-01
CH3OH	9.43E-03	0	0	4.27E-03	5.87E-03	1.43E-03	2.10E-02
S	8.90E-03	0	0	4.03E-03	5.54E-03	1.35E-03	1.98E-02
SO2	2.80E-02	0	0	1.27E-02	1.74E-02	4.25E-03	6.23E-02
O2	6.21E-03	0	0	2.81E-03	3.87E-03	9.43E-04	1.38E-02
NH3	2.31E-03	0	0	1.05E-03	1.44E-03	3.51E-04	5.15E-03

Table A.32

FIRST REHEATER AND FIRST REACTOR STAGE
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE CLAUS TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	1
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	1
Heat - Exchangers (Heating Side)	1
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	3
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO2	42	1852	3.24E-01
H2O	15	262	4.58E-02
H2S	23	788	1.38E-01
N2	63	1764	3.08E-01
CH3OH	9	288	5.03E-02
S	0	0	0
SO2	9	570	9.96E-02
O2	4	126	2.21E-02
NH3	4	71	1.23E-02
TOTAL FLOW	169	5721	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0.104	0.00083	0.0017
QUANTITY	52	0	0	1	218	26

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO2	9.43E-02	0	0	3.37E-02	5.87E-02	1.43E-02	2.01E-01
H2O	1.33E-02	0	0	4.77E-03	8.31E-03	2.03E-03	2.85E-02
H2S	4.01E-02	0	0	1.43E-02	2.50E-02	6.09E-03	8.55E-02
N2	8.98E-02	0	0	3.21E-02	5.59E-02	1.36E-02	1.91E-01
CH3OH	1.47E-02	0	0	5.24E-03	9.12E-03	2.22E-03	3.12E-02
S	0	0	0	0	0	0	0
SO2	2.90E-02	0	0	1.04E-02	1.80E-02	4.40E-03	6.18E-02
O2	6.43E-03	0	0	2.30E-03	4.00E-03	9.77E-04	1.37E-02
NH3	3.59E-03	0	0	1.28E-03	2.24E-03	5.45E-04	7.65E-03

Table A.33

SECOND REHEATER AND SECOND REACTOR STAGE
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE CLAUS TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	1
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	1
Heat - Exchangers (Heating Side)	1
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	2
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO2	42	1852	3.67E-01
H2O	29	516	1.02E-01
H2S	9	309	6.13E-02
N2	63	1764	3.50E-01
CH3OH	9	288	5.71E-02
S	0	0	0
SO2	2	119	2.36E-02
O2	4	126	2.51E-02
NH3	4	71	1.40E-02
TOTAL FLOW	162	5045	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0.104	0.00083	0.0017
QUANTITY	46	0	0	1	193	23

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO2	9.46E-02	0	0	3.82E-02	5.89E-02	1.44E-02	2.06E-01
H2O	2.63E-02	0	0	1.06E-02	1.64E-02	4.00E-03	5.73E-02
H2S	1.58E-02	0	0	6.38E-03	9.83E-03	2.40E-03	3.44E-02
N2	9.01E-02	0	0	3.64E-02	5.61E-02	1.37E-02	1.96E-01
CH3OH	1.47E-02	0	0	5.94E-03	9.15E-03	2.23E-03	3.20E-02
S	0	0	0	0	0	0	0
SO2	6.08E-03	0	0	2.45E-03	3.78E-03	9.22E-04	1.32E-02
O2	6.45E-03	0	0	2.61E-03	4.02E-03	9.80E-04	1.41E-02
NH3	3.60E-03	0	0	1.45E-03	2.24E-03	5.47E-04	7.85E-03

Table A.34

THIRD REHEATER AND REACTOR STAGE
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE CLAUS TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	1
Horizontal Vessles	1
Storage Tanks	0
Pressure Relief Valves	1
Heat - Exchangers (Heating Side)	1
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	2
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO2	42	1852	3.78E-01
H2O	32	570	1.16E-01
H2S	6	206	4.21E-02
N2	63	1764	3.60E-01
CH3OH	9	288	5.88E-02
S	0	0	0
SO2	0	22	4.44E-03
O2	4	126	2.58E-02
NH3	4	71	1.44E-02
TOTAL FLOW	160	4900	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0.104	0.00083	0.0017
QUANTITY	67	0	0	1	281	34

COMPONENT	EMISSIONS FROM:						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO2	1.42E-01	0	0	3.93E-02	8.83E-02	2.15E-02	2.91E-01
H2O	4.37E-02	0	0	1.21E-02	2.72E-02	6.63E-03	8.96E-02
H2S	1.58E-02	0	0	4.38E-03	9.84E-03	2.40E-03	3.24E-02
N2	1.35E-01	0	0	3.74E-02	8.41E-02	2.05E-02	2.77E-01
CH3OH	2.21E-02	0	0	6.11E-03	1.37E-02	3.35E-03	4.52E-02
S	0	0	0	0	0	0	0
SO2	1.67E-03	0	0	4.62E-04	1.04E-03	2.53E-04	3.42E-03
O2	9.68E-03	0	0	2.68E-03	6.03E-03	1.47E-03	1.99E-02
NH3	5.40E-03	0	0	1.50E-03	3.36E-03	8.20E-04	1.11E-02

Table A.35

SULFUR CONDENSER
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE CLAUS TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	0
Horizontal Vessles	1
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	4
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO2	154	6792	3.34E-01
H2O	107	1931	9.49E-02
H2S	31	1060	5.21E-02
N2	250	6991	3.44E-01
CH3OH	33	1056	5.19E-02
S	32	1037	5.10E-02
SO2	11	710	3.49E-02
O2	16	506	2.49E-02
NH3	15	259	1.27E-02
TOTAL FLOW	650	20341	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0	0.00083	0.0017
QUANTITY	45	0	0	0	189	23

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO2	8.41E-02	0	0	0	5.24E-02	1.28E-02	1.49E-01
H2O	2.39E-02	0	0	0	1.49E-02	3.63E-03	4.24E-02
H2S	1.31E-02	0	0	0	8.17E-03	1.99E-03	2.33E-02
N2	8.66E-02	0	0	0	5.39E-02	1.31E-02	1.54E-01
CH3OH	1.31E-02	0	0	0	8.14E-03	1.99E-03	2.32E-02
S	1.28E-02	0	0	0	8.00E-03	1.95E-03	2.28E-02
SO2	8.80E-03	0	0	0	5.48E-03	1.34E-03	1.56E-02
O2	6.26E-03	0	0	0	3.90E-03	9.51E-04	1.11E-02
NH3	3.21E-03	0	0	0	2.00E-03	4.87E-04	5.69E-03

BEAVON PLANT

The flowsheet for the Beavon Plant along with the information needed for the stream estimations were taken from the <u>Gas Process Handbook '84</u>, <u>Hydrocarbon Processing</u>, April 1984, p. 88.

Table A.36

BEAVON PLANT OVERALL FUGITIVE EMISSIONS FOR ONE TRAIN

COMPONENT	EMISSIONS FROM:						TOTAL
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open-Ended Lines (kg/hr)	EMISSIONS (kg/hr)
CO2	9.17E-01	7.52E-02	0	0	5.12E-01	1.25E-01	1.63
O2	9.96E-02	5.13E-03	0	9.84E-03	5.31E-02	1.29E-02	0.18
S	1.49E-01	0	0	2.61E-02	7.32E-02	1.78E-02	0.27
H2O	2.55E+00	2.36E-02	0	3.98E-01	1.27E+00	3.10E-01	4.55
H2S	3.20E-01	7.45E-03	0	4.77E-02	1.63E-01	3.98E-02	0.58
N2	1.74E+00	0	0	1.42E-01	9.11E-01	2.22E-01	3.08
NH3	3.49E-02	2.86E-03	0	0	1.95E-02	4.76E-03	0.06
CH3OH	1.43E-01	1.17E-02	0	0	7.96E-02	1.94E-02	0.25

The following tables (A.37-A.46) are the actual estimations made for the Beavon Plant in Base Case 1.

Table A.37

ESTIMATION OF FUGITIVE EMISSIONS FOR THE BEAVON PLANT

BEAVON PLANT	
QUANTITY	EQUIPMENT TYPE
4	Pumps
16	Vertical Vessles
6	Horizontal Vessles
2	Storage Tanks
6	Pressure Relief Valves
2	Heat - Exchangers (Heating Side)
2	Heat - Exchangers (Cooling Side)
0	Loading or Unloading Point
42	Flow Transmitters
0	Turbine Meter and Prover Connection

QUANTITY	ACTUAL EQUIPMENT
2	Preheater
2	Hydrolysis Reactor
4	Boilers
4	Pumps
2	Desuperheater Contact Condenser
2	Venturi Scrubber-Stripper
8	Pressure Relief Valves
4	Oxidizer Tanks
2	Slurry Tank
2	Balance Tank
2	Separation Wash and Reslurry
2	Sulfur Collector Drum
46	Flow Transmitters

QUANTITY	ESTIMATED EQUIPMENT
442	Valves
221	Open - Ended Lines
1856	Flanges

QUANTITY	EQUIPMENT WITH FUGITIVES
442	Valves
4	Pumps
0	Compressors
8	Pressure Relief Valves
1856	Flanges
221	Open - Ended Lines

Table A.38

FEED COOLER
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE BEAVON TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	0
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	1
Loading or Unloading Point	0
Flow Transmitters	2
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO2	42	1852	3.81E-01
O2	4	126	2.60E-02
S	0	0	0
H2O	32	582	1.20E-01
H2S	5	184	3.77E-02
N2	63	1764	3.62E-01
NH3	4	71	1.45E-02
CH3OH	9	288	5.92E-02
TOTAL FLOW	160	4867	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0	0.00083	0.0017
QUANTITY	29	0	0	0	122	15

COMPONENT	EMISSIONS FROM:						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO2	6.18E-02	0	0	0	3.85E-02	9.38E-03	1.10E-01
O2	4.22E-03	0	0	0	2.63E-03	6.40E-04	7.48E-03
S	0	0	0	0	0	0	0
H2O	1.94E-02	0	0	0	1.21E-02	2.95E-03	3.45E-02
H2S	6.13E-03	0	0	0	3.81E-03	9.30E-04	1.09E-02
N2	5.89E-02	0	0	0	3.66E-02	8.93E-03	1.04E-01
NH3	2.35E-03	0	0	0	1.47E-03	3.57E-04	4.18E-03
CH3OH	9.61E-03	0	0	0	5.98E-03	1.46E-03	1.70E-02

Table A.39

DESUPERHEATER CONTACT CONDENSER (liquid lines)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE BEAVON TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	2
Vertical Vessles	1
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	1
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	5
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO2	42	1852	3.81E-01
O2	4	126	2.60E-02
S	0	0	0
H20	32	582	1.20E-01
H2S	5	184	3.77E-02
N2	63	1764	3.62E-01
NH3	4	71	1.45E-02
CH3OH	9	288	5.92E-02
TOTAL FLOW	160	4867	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0071	0.0494	0	0	0.00083	0.0017
QUANTITY	83	2	0	0	349	42

COMPONENT	EMISSIONS FROM:						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO2	2.24E-01	3.76E-02	0	0	1.10E-01	2.69E-02	3.99E-01
O2	1.53E-02	2.57E-03	0	0	7.51E-03	1.83E-03	2.72E-02
S	0	0	0	0	0	0	0
H20	7.05E-02	1.18E-02	0	0	3.48E-02	8.44E-03	1.25E-01
H2S	2.22E-02	3.73E-03	0	0	1.09E-02	2.68E-03	3.95E-02
N2	2.14E-01	3.58E-02	0	0	1.05E-01	2.58E-02	3.80E-01
NH3	8.54E-03	1.43E-03	0	0	4.19E-03	1.02E-03	1.52E-02
CH3OH	3.49E-02	5.85E-03	0	0	1.71E-02	4.17E-03	6.20E-02

Table A.40

DESUPERHEATER CONTACT CONDENSER (vapor lines)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE BEAVON TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	1
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	2
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO2	42	1852	3.81E-01
O2	4	126	2.60E-02
S	0	0	0
H2O	32	582	1.20E-01
H2S	5	184	3.77E-02
N2	63	1764	3.62E-01
NH3	4	71	1.45E-02
CH3OH	9	288	5.92E-02
TOTAL FLOW	160	4867	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0	0.00083	0.0017
QUANTITY	35	0	0	0	147	18

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO2	7.46E-02	0	0	0	4.64E-02	1.13E-02	1.32E-01
O2	5.09E-03	0	0	0	3.17E-03	7.73E-04	9.03E-03
S	0	0	0	0	0	0	0
H2O	2.34E-02	0	0	0	1.46E-02	3.56E-03	4.16E-02
H2S	7.39E-03	0	0	0	4.60E-03	1.12E-03	1.31E-02
N2	7.10E-02	0	0	0	4.42E-02	1.08E-02	1.26E-01
NH3	2.84E-03	0	0	0	1.77E-03	4.31E-04	5.04E-03
CH3OH	1.16E-02	0	0	0	7.22E-03	1.76E-03	2.06E-02

Table A.41

VENTURI SCRUBBER / STRIPPER *(vapor line)*
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE BEAVON TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	2
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	0
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO2	42	1852	3.81E-01
O2	4	126	2.60E-02
S	0	0	0
H20	32	582	1.20E-01
H2S	5	184	3.77E-02
N2	63	1764	3.62E-01
NH3	4	71	1.45E-02
CH3OH	9	288	5.92E-02
TOTAL FLOW	160	4867	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0056	0	0	0	0.00083	0.0017
QUANTITY	46	0	0	0	193	23

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO2	9.80E-02	0	0	0	6.10E-02	1.49E-02	1.74E-01
O2	6.69E-03	0	0	0	4.16E-03	1.02E-03	1.19E-02
S	0	0	0	0	0	0	0
H20	3.08E-02	0	0	0	1.92E-02	4.68E-03	5.47E-02
H2S	9.72E-03	0	0	0	6.05E-03	1.47E-03	1.72E-02
N2	9.34E-02	0	0	0	5.81E-02	1.42E-02	1.66E-01
NH3	3.73E-03	0	0	0	2.32E-03	5.67E-04	6.62E-03
CH3OH	1.52E-02	0	0	0	9.49E-03	2.31E-03	2.70E-02

Table A.42

VENTURI SCRUBBER / STRIPPER (liquid lines)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE BEAVON TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	2
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	5
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO_2	0	0	0
O_2	0	0	0
S	0	0	0
H_2O	20	360	5.81E-01
H_2S	1	34	5.49E-02
N_2	8	225	3.64E-01
NH_3	0	0	0
CH_3OH	0	0	0
TOTAL FLOW	29	619	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0071	0	0	0	0.00083	0.0017
QUANTITY	76	0	0	0	319	38

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO_2	0	0	0	0	0	0	0
O_2	0	0	0	0	0	0	0
S	0	0	0	0	0	0	0
H_2O	3.14E-01	0	0	0	1.54E-01	3.75E-02	5.05E-01
H_2S	2.96E-02	0	0	0	1.45E-02	3.55E-03	4.77E-02
N_2	1.96E-01	0	0	0	9.64E-02	2.35E-02	3.16E-01
NH_3	0	0	0	0	0	0	0
CH_3OH	0	0	0	0	0	0	0

Table A.43

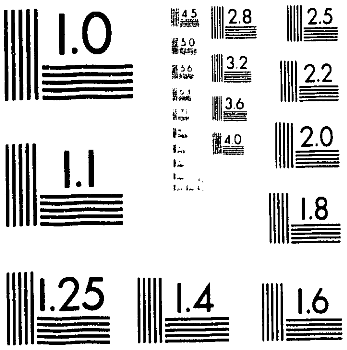
OXIDIZER TANK (liquid)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE BEAVON TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	2
Horizontal Vessles	0
Storage Tanks	0
Pressure Relief Valves	1
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	1
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO2	0	0	0
O2	2	69	4.73E-02
S	0	0	0
H20	52	942	6.48E-01
H2S	6	218	1.50E-01
N2	8	225	1.55E-01
NH3	0	0	0
CH3OH	0	0	0
TOTAL FLOW	69	1454	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0071	0	0	0.104	0.00083	0.0017
QUANTITY	55	0	0	1	231	28

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO2	0	0	0	0	0	0	0
O2	1.85E-02	0	0	4.92E-03	9.07E-03	2.21E-03	3.47E-02
S	0	0	0	0	0	0	0
H20	2.53E-01	0	0	6.74E-02	1.24E-01	3.03E-02	4.75E-01
H2S	5.84E-02	0	0	1.56E-02	2.87E-02	7.00E-03	1.10E-01
N2	6.05E-02	0	0	1.61E-02	2.97E-02	7.25E-03	1.14E-01
NH3	0	0	0	0	0	0	0
CH3OH	0	0	0	0	0	0	0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1.4
1.6

2 of 2

Table A.44

SLURRY TANK AND WASH (liquid)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE BEAVON TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	0
Horizontal Vessles	1
Storage Tanks	1
Pressure Relief Valves	1
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	2
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO2	0	0	0
02	0	0	0
S	5	173	1.26E-01
H20	52	942	6.86E-01
H2S	1	34	2.47E-02
N2	8	225	1.64E-01
NH3	0	0	0
CH3OH	0	0	0
TOTAL FLOW	67	1375	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0071	0	0	0.104	0.00083	0.0017
QUANTITY	49	0	0	1	206	25

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO2	0	0	0	0	0	0	0
02	0	0	0	0	0	0	0
S	4.37E-02	0	0	1.31E-02	2.15E-02	5.24E-03	8.35E-02
H20	2.39E-01	0	0	7.13E-02	1.17E-01	2.86E-02	4.55E-01
H2S	8.61E-03	0	0	2.57E-03	4.23E-03	1.03E-03	1.64E-02
N2	5.71E-02	0	0	1.71E-02	2.80E-02	6.83E-03	1.09E-01
NH3	0	0	0	0	0	0	0
CH3OH	0	0	0	0	0	0	0

Table A.45

BALANCE TANK (liquid)
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE BEAVON TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	0
Horizontal Vessles	1
Storage Tanks	0
Pressure Relief Valves	1
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	1
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO2	0	0	0
O2	0	0	0
S	0	0	0
H2O	20	360	5.81E-01
H2S	1	34	5.49E-02
N2	8	225	3.64E-01
NH3	0	0	0
CH3OH	0	0	0
TOTAL FLOW	29	619	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0071	0	0	0.104	0.00083	0.0017
QUANTITY	30	0	0	1	126	15

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO2	0	0	0	0	0	0	0
O2	0	0	0	0	0	0	0
S	0	0	0	0	0	0	0
H2O	1.24E-01	0	0	6.04E-02	6.08E-02	1.48E-02	2.60E-01
H2S	1.17E-02	0	0	5.71E-03	5.74E-03	1.40E-03	2.45E-02
N2	7.75E-02	0	0	3.78E-02	3.81E-02	9.28E-03	1.63E-01
NH3	0	0	0	0	0	0	0
CH3OH	0	0	0	0	0	0	0

Table A.46

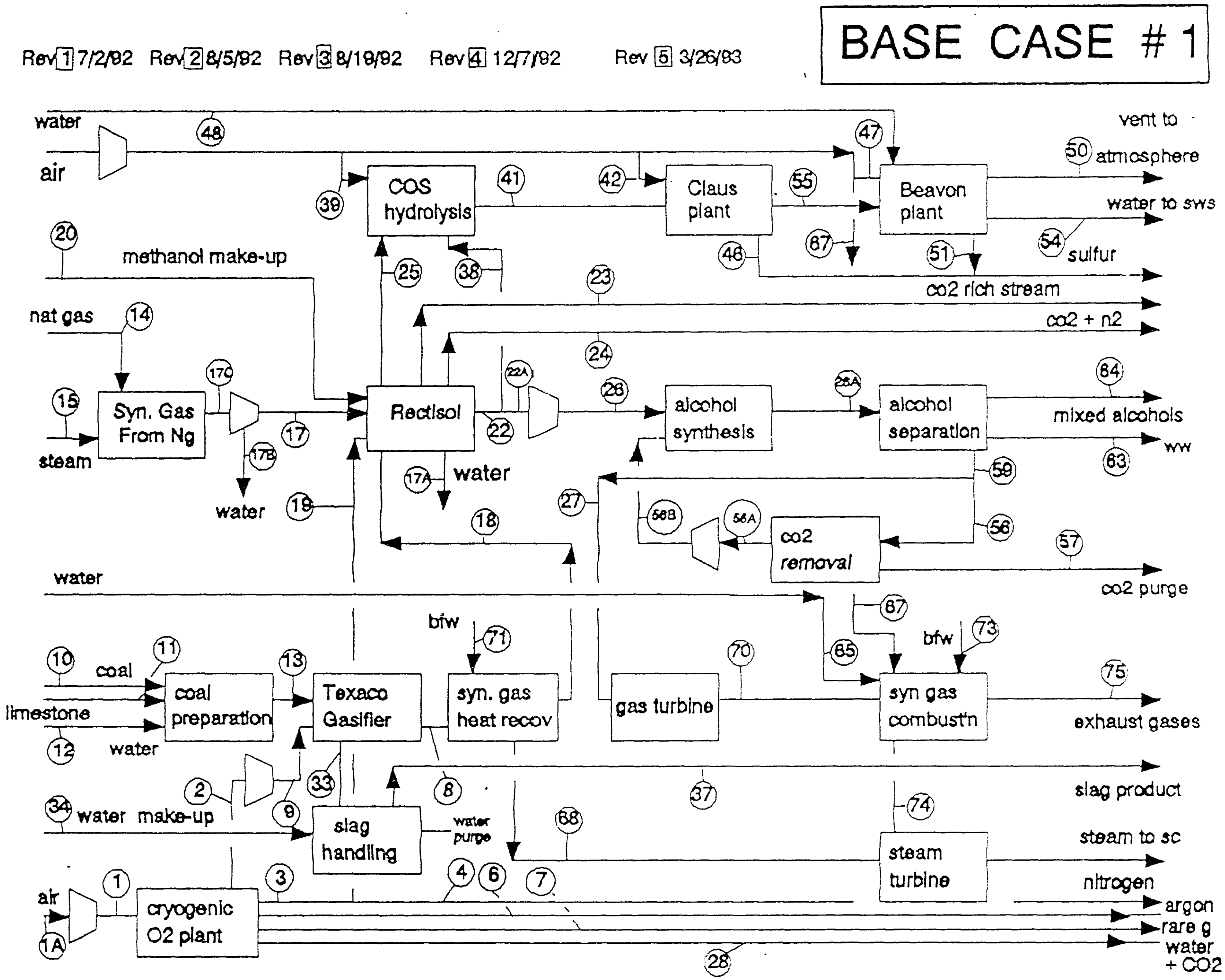
WATER - SULFUR SEPARTOR
ESTIMATION OF FUGITIVE EMISSIONS FOR ONE BEAVON TRAIN

EQUIPMENT TYPE	QUANTITY
Pumps	0
Vertical Vessles	0
Horizontal Vessles	1
Storage Tanks	0
Pressure Relief Valves	0
Heat - Exchangers (Heating Side)	0
Heat - Exchangers (Cooling Side)	0
Loading or Unloading Point	0
Flow Transmitters	3
Turbine Meter and Prover Connection	0

FLOW SUMMARY	kgmol/hr	kg/hr	mass fraction
CO2	0	0	0
O2	0	0	0
S	5	173	1.11E-01
H20	62	1122	7.22E-01
H2S	1	34	2.19E-02
N2	8	225	1.45E-01
NH3	0	0	0
CH3OH	0	0	0
TOTAL FLOW	77	1555	

EQUIPMENT WITH FUGITIVES	Valves	Pumps	Compressors	Pressure Relief Valves	Flanges	Open - Ended Lines
EMISSION FACTOR	0.0071	0	0	0	0.00083	0.0017
QUANTITY	39	0	0	0	184	20

COMPONENT	EMISSIONS FROM :						TOTAL EMISSIONS (kg/hr)
	Valves (kg/hr)	Pumps (kg/hr)	Compressors (kg/hr)	Pressure Relief Valves (kg/hr)	Flanges (kg/hr)	Open - Ended Lines (kg/hr)	
CO2	0	0	0	0	0	0	0
O2	0	0	0	0	0	0	0
S	3.08E-02	0	0	0	1.51E-02	3.68E-03	4.96E-02
H20	2.00E-01	0	0	0	9.82E-02	2.39E-02	3.22E-01
H2S	6.06E-03	0	0	0	2.97E-03	7.25E-04	9.75E-03
N2	4.02E-02	0	0	0	1.97E-02	4.81E-03	6.47E-02
NH3	0	0	0	0	0	0	0
CH3OH	0	0	0	0	0	0	0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Rev 1 7/2/82 Rev 2 8/5/82 Rev 3 8/19/82 Rev 4 12/7/82 Rev 5 3/26/83
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air
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39
COS hydrolysis
41
42
Claus plant
55
47
Beavon plant
vent to atmosphere
50
water to sws
54
sulfur
67
46
51
co2 rich stream
20
methanol make-up
25
38
23
co2 + n2
24
nat gas
14
15
steam
Syn. Gas From Ng
17C
17B
17
water
Rectisol
22
22A
28
alcohol synthesis
28A
alcohol separation
64
mixed alcohols
63
ww
17A
water
19
18
27
59
56B
56A
co2 removal
56
57
co2 purge
water
bfw
71
87
65
bfw
73
10
coal
11
coal preparation
13
Texaco Gasifier
syn. gas heat recov
70
gas turbine
syn gas combust'n
75
exhaust gases
limestone
12
water
2
33
8
37
slag product
34
water make-up
9
slag handling
water purge
68
74
steam turbine
steam to sc
air
1A
1
cryogenic O2 plant
3
4
6
7
nitrogen
argon
rare g
water + CO2
28

Figure A.1

Base Case 1	001	001A	002	003	004	006	008	009	010	011
Ar	118.2	118.2	0.0	0.0	0.0	118.2	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5618.7	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H5OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H7OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5H11OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	0.0	4105.2	0.0	0.0	0.0
CO2	4.1	4.1	0.0	0.0	0.0	0.0	1483.4	0.0	0.0	0.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	3.5	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.6
H2	0.0	0.0	0.0	0.0	0.0	0.0	3026.7	0.0	2296.0	0.0
H2O	305.5	305.5	0.0	0.0	0.0	0.0	3893.0	0.0	64.7	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	71.9	0.0	0.0	0.0
N2	9898.3	9898.3	0.0	9898.3	7161.4	0.0	45.6	0.0	49.7	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	8.3	0.0	0.0	0.0
O2	2661.1	2661.1	2661.1	0.0	0.0	0.0	0.0	2661.1	442.5	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	75.5	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	105.2	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	26.6	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	12987.2	12987.2	2661.1	9898.3	7161.4	118.2	12637.6	2661.1	8652.3	4.6
kg/hr	372715.0	372715.0	85155.2	277152.4	200519.2	4728.0	260630.7	85155.2	101879.0	460.0
Temp.(C)	262.0	25.0	25.0	25.0	25.0	25.0	1300.0	40.0	25.0	25.0
Press.(KPA)	517.1	103.4	517.1	517.1	517.1	517.1	8135.8	8135.8	103.4	103.4

Table A.47

	012	013	014	015	017	017A	017B	17C	018	019
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	5618.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H5OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H7OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5H11OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	567.3	0.0	567.4	0.0	4105.2	0.0
CO2	0.0	0.0	0.0	0.0	132.4	0.0	132.8	0.0	1483.4	0.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.5	0.0
CaCO3	0.0	4.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	2296.0	0.0	0.0	2233.2	0.0	2233.3	0.0	3026.7	0.0
H2O	4696.7	4761.4	0.0	1656.0	6.6	3899.6	823.1	776.5	3893.0	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	72.0	0.0
N2	0.0	49.7	0.0	0.0	0.0	0.0	0.0	0.0	45.6	2736.9
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.3	0.0
O2	0.0	442.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	75.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	105.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	700.7	0.0	4.8	0.0	0.5	0.0	26.6	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	4696.7	13353.6	0.0	1656.0	2939.5	3899.6	3756.6	776.5	12637.7	2736.9
kg/hr	84540.6	186879.6	11211.2	29808.0	26372.2	70192.8	41020.8	13977.0	260634.1	76633.2
Temp.(C)	25.0	25.0	135.0	300.0	25.0	25.0	926.9	25.0	25.0	25.0
Press.(KPA)	103.4	8135.8	200.0	200.0	8106.0	8106.0	202.0	202.0	8135.8	517.1

Table A.47 (Continued)

	020	022	022A	023	024	025	026	026A	027	028
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	18.0	0.0	0.0	0.0	0.0	18.0	0.0	622.5	0.0	0.0
C2H5OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	649.4	0.0	0.0
C3H7OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	143.7	0.0	0.0
C4H9OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	36.2	0.0	0.0
C5H11OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	15.0	0.0	0.0
CO	0.0	4672.5	4625.8	0.0	0.0	0.0	4625.8	6937.6	0.0	0.0
CO2	0.0	0.0	0.0	969.5	565.5	80.7	0.0	1480.0	0.0	4.1
COS	0.0	0.0	0.0	0.0	0.0	3.5	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	5260.0	5207.3	0.0	0.0	0.0	5207.4	8332.7	0.0	0.0
H2O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	138.8	0.0	305.5
H2S	0.0	0.0	0.0	0.0	0.0	72.0	0.0	0.0	0.0	0.0
N2	0.0	0.0	0.0	0.0	2782.5	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	8.3	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	17.9	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	11.8	0.0	0.0
CH4	0.0	27.2	26.9	0.0	0.0	0.0	26.9	464.0	464.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	17.3	17.3	0.0
kmol/hr	18.0	9932.5	9833.1	969.5	3348.0	182.5	9833.2	18385.6	0.0	309.6
kg/hr	576.0	141785.2	140367.4	42658.0	102792.0	6715.9	140368.2	351255.8	7943.0	5679.4
Temp.(C)	25.0	25.0	25.0	25.0	25.0	25.0	310.0	310.0	50.0	25.0
Press.(KPA)	103.4	8106.0	8106.0	8106.0	8106.0	8106.0	14000.0	12666.0	12666.0	517.1

Table A.47 (Continued)

	033	034	036	037	038	039	041	042	045	046
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	18.0	0.0	18.0	0.0
C2H5OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H7OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5H11OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	46.7	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	0.0	78.8	0.0	80.7	0.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	4.6	0.0	0.0	4.6	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	52.6	0.0	0.0	0.0	0.0	0.0
H2O	0.0	251.2	251.2	0.0	0.0	0.0	0.0	0.0	64.7	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	60.1	0.0	10.6	0.0
N2	0.0	0.0	0.0	0.0	0.0	89.2	0.0	112.0	126.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	6.6	0.0	8.3	0.0
O2	0.0	0.0	0.0	0.0	0.0	32.0	0.0	40.2	7.9	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	64.8
Al2O3	105.2	0.0	0.0	105.2	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.3	0.0	0.0	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.3	0.0	0.0	0.0	0.0	0.0
kmol/hr	109.8	251.2	251.2	109.8	99.3	121.2	163.5	152.2	316.2	64.8
kg/hr	11190.4	4521.6	4521.6	11190.4	1426.0	3520.4	6198.8	4422.4	9573.7	2073.6
Temp.(C)	1300.0	25.0	156.0	156.0	25.0	25.0	25.0	25.0	370.0	370.0
Press.(KPA)	8135.8	3447.4	3000.0	103.4	8106.0	15.0	15.0	103.4	103.4	103.4

Table A.47 (Continued)

	047	048	050	051	054	056	056A	056B	057	059
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	18.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H5OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H7OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5H11OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	6937.6	6937.6	6937.6	0.0	6937.6
CO2	0.0	0.0	84.2	0.0	0.0	1480.0	0.0	0.0	1480.0	1480.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0	8329.5	8329.5	8329.5	0.0	8329.5
H2O	0.0	20.0	0.0	0.0	72.0	0.0	0.0	0.0	0.0	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	16.1	0.0	142.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	8.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	4.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	7.2	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	464.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	17.3
kmol/hr	20.4	20.0	252.6	7.2	72.0	16747.1	15267.1	15267.1	1480.0	16747.1
kg/hr	588.4	360.0	8400.7	230.4	1296.0	276031.8	210911.8	210911.8	65120.0	283974.8
Temp.(C)	25.0	25.0	370.0	25.0	370.0	310.0	310.0	310.0	25.0	310.0
Press.(KPA)	103.4	15.0	103.4	103.4	103.4	12666.0	12666.0	14185.0	12666.0	12666.0

Table A.47 (Continued)

	063	064	065	067	068	070	071	073	074	075
Ar	0.0	0.0	0.0	62.0	0.0	0.0	0.0	0.0	0.0	62.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	622.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H5OH	0.0	649.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H7OH	0.0	143.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	36.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5H11OH	0.0	15.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	498.6
COS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	138.7	0.0	422.5	0.0	9626.4	0.0	9626.4	6200.0	6200.0	1402.4
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	0.0	0.0	0.0	4827.6	0.0	0.0	0.0	0.0	0.0	4827.6
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	1292.0	0.0	0.0	0.0	0.0	0.0	303.4
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	17.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	11.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	464.0	0.0	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	17.3	0.0	0.0	0.0	0.0
kmol/hr	168.4	1466.8	422.5	6181.6	9626.4	0.0	9626.4	6200.0	6200.0	7094.0
kg/hr	4859.6	62413.2	7605.0	178996.8	173275.2	7943.0	173275.2	111600.0	111600.0	194543.2
Temp.(C)	25.0	25.0	25.0	25.0	482.0	25.0	20.0	20.0	482.2	25.0
Press.(KPA)	12666.0	12666.0	103.4	103.4	10000.0	101.3	10000.0	10000.0	10400.0	101.3

Table A.47 (Continued)