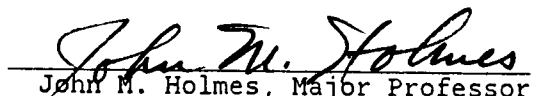
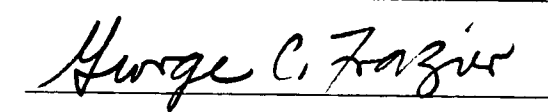


To the Graduate Council:

I am submitting herewith a thesis written by Sambamurty Raju Dantuluri entitled "Computer Aided Study of Coal Utilization in The United States Ammonia Industry." I have examined the final copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Chemical Engineering.


John M. Holmes, Major Professor

We have read this thesis
and recommend its acceptance:

Accepted for the Council:


The Graduate School

COMPUTER AIDED STUDY OF COAL UTILIZATION
IN THE UNITED STATES AMMONIA INDUSTRY

A Thesis
Presented for the
Master of Science
Degree
The University of Tennessee, Knoxville

Sambamurty Raju Dantuluri

March 1985

To my
Wife Krishna Kumari
And kids
Ravi and Surendra

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ABSTRACT

A study is made to develop possible alternatives to replace expensive natural gas for manufacturing ammonia. The alternative energy source coal, has been considered to replace natural gas as feedstock as well as fuel for the primary reformer in a conventional steam reforming process for the production of ammonia. Natural gas feedstock is replaced by generating synthesis gas using a coal-fed Texaco gasifier. A Coal fired Atmospheric Fluidized Bed Combustor (AFBC) reformer and Medium Btu Gas (MBG) fuel are considered as alternative arrangements.

The Advanced System for Process Engineering (ASPEN) computer simulation is utilized to perform mass and energy balances for different process flow-schemes. The economics of ammonia production with various process alternatives is developed with the help of CASHFLOW computer program for discounted cash flow.

The future year production costs of ammonia with alternative arrangements were compared with the costs for conventional process to find out the break even point in time. The AFBC reformer arrangement was found to be economically attractive whereas MBG fuel for the reformer was observed to be too expensive. Coal as a feedstock for ammonia production is expected to be economical during the early years of next decade, but not in immediate future.

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CHAPTER I

INTRODUCTION

Ammonia is one of the leading energy based chemical products manufactured in all developed countries. A major portion of the ammonia produced in these countries is being consumed by the fertilizer industry. The growth in agriculture in any country can be measured by the growth in fertilizer use in that country and in turn by the production of ammonia. In the US, agriculture is the largest industry with its assets ammounting to about three fifths of the capital assets of all manufacturing corporations (1). Therefore, the production of ammonia is vital to the consumers of agriculture products and those employed by the high agribusiness. Natural gas is the most commonly used feedstock for ammonia production in the US. There are over 100 ammonia plants in the US, having the capability of producing over 20 million tons of ammonia per year. On an average, these plants will consume over 700 billion scf of natural gas per year (2). A study indicates that at least 95 percent of manufacturers in the US utilize natural gas as the feedstock (3). It's obvious from above that the ammonia industry in the US relies heavily on natural gas as it's major feedstock.

However, the rising cost of natural gas is one of the many reasons for the shut down of some ammonia plants recently (33). In less than ten years the cost of natural gas has risen more than ten-fold whereas from 1950-1970 the price only doubled. Figure 1.1 depicts the trend of delivered natural gas prices in recent years.

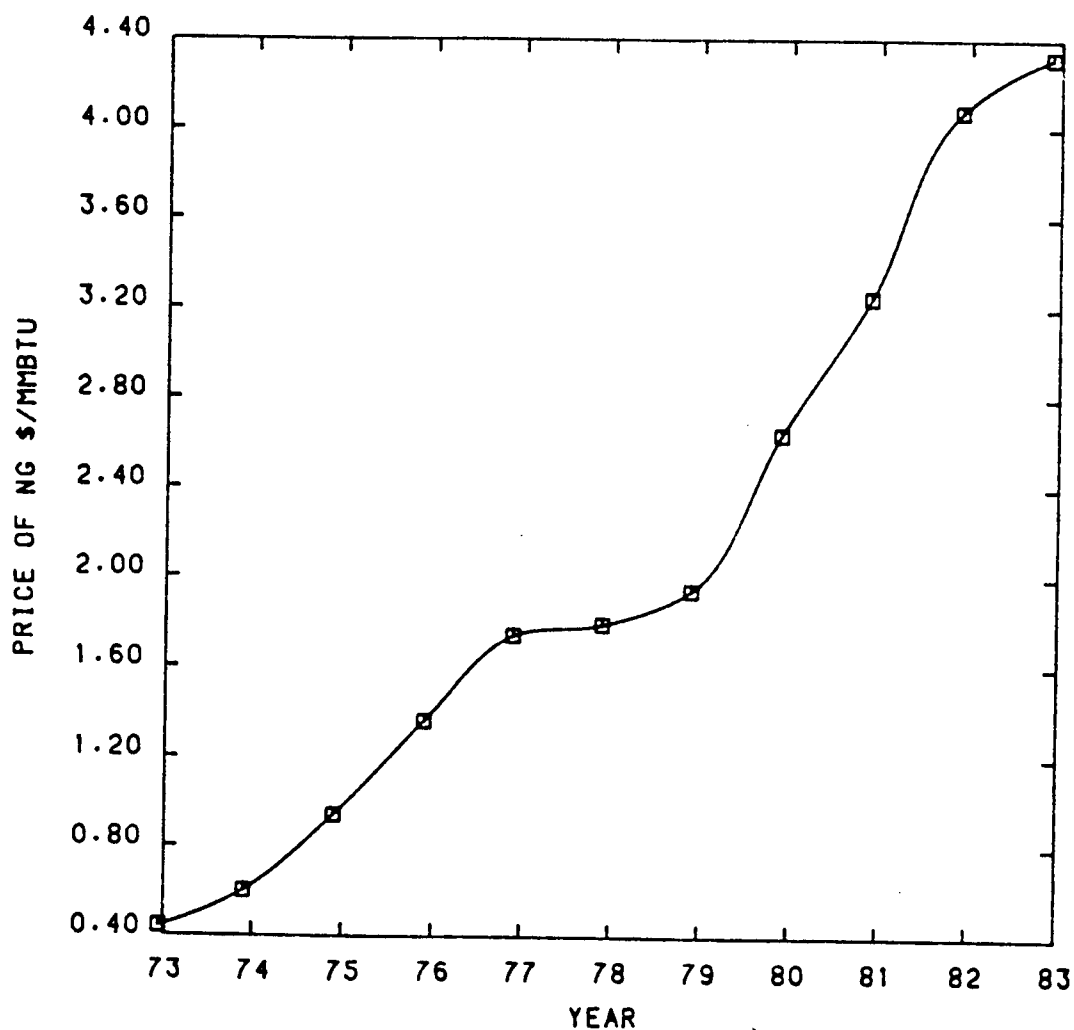


Figure 1.1. Industrial natural gas price (current dollars) in recent years

Source: Monthly Gas Utility Statistical Report, Dec. 1982

Due to the low probability that large new oil and gas reserves will be discovered, the future prices of oil and gas are expected to increase rapidly. Since 1978, gas prices have been regulated by the Natural Gas Policy Act (NGPA), to control the prices of natural gas. However, natural gas prices were locked into an upward course under NGPA at a time when oil prices were relatively weak. The act is pending deregulation in 1985. The situation is expected to become increasingly unstable with gas price deregulation and the price of natural gas is expected to rise in the latter part of the decade (58).

The price of natural gas plays a vital role in determining the production cost of ammonia. A recent study indicates that natural gas for feedstock and fuel will account for more than 83 percent of the product cost by the year 1985, compared to about 60 percent at present (4). It is obvious from the above mentioned conditions that the ammonia industry will experience a critical period during the next decade to maintain profitability in the light of increasingly expensive natural gas supplies.

In the face of rising prices of natural gas, ammonia producers are looking for energy saving measures and alternate fuels. At present, the US energy policy is also directed towards limiting imports and increasing the security of energy supply (2). At this present situation one attractive alternative source of energy, with high potential for satisfying the increasing demands of energy is coal. The US coal reserves are tremendous such that reliance on domestic coal alone will secure it's energy supply. Recent

estimates project the production of coal to increase on the order of 75 percent or more by the year 2000 (5). This assures the availability of this new source of energy over a long period of time. Table 1.1 shows the past and projected demand and production of coal in the US. Increasing demand of coal for the production of synthetic fuels is included in these projections. The price of coal is relatively stable compared to the price of natural gas. The increase in coal price in recent years is much lower compared to that of natural gas. For example, in the last five year period, the natural gas price has gone up by 140 percent compared to 60 percent for the coal (24).

The present study has been made to focus the energy savings and develop the economics for ammonia production with coal as an alternate fuel and feedstock. Out of the total quantity of natural gas consumed in ammonia industry, one third is being utilized as fuel for the primary reformers. This study considers coal combustion in an atmospheric fluidized bed combustor as the first alternative for natural gas fuel. The economics with this arrangement has been studied. Medium BTU gas generated from a Babcock and Wilcox gasifier has also been looked into as a second alternative for the fuel. The economics of producing ammonia in future years with this fuel has been developed. Coal is also being considered as a potential feedstock for ammonia production and the economics with this alternate feedstock is studied in comparison with the conventional steam reforming process of natural gas.

TABLE 1.1
US COAL DEMAND AND PRODUCTION
(millions of tons)

Year	Coal	C O A L D E M A N D				
	mined	Conventional markets		Export	Syn. fuels	Total
1978	665	625		41	0	666
1979	776	677		65	0	742
1980	825	715		84	0	799
1981	800	750		87	0	837
1985	1011	892		80	4	976
1990	1321	1207		100	14	1321

Source: Hydrocarbon Processing, Jan. 1982, p. 19.

In all the above studies, the material and energy balances were performed using the Advanced System for Process ENgineering (ASPEN) which is a comprehensive computer program developed for process and economic evaluations by the US Dept.of Energy (32). The economics are being evaluated with help of Discounted Cash Flow(DCF) computer program (21).

CHAPTER II

REVIEW OF LITERATURE

2.1 Coal--Ammonia

Raw materials used for making ammonia include natural gas, coal, coke, lignite, crude petroleum, fuel oil, naphtha, refinery gas, cokeoven gas and by-product hydrogen from chlorine/caustic cells. It is reported that even wood was used as raw material for several years in India and the USSR during the 1920s (6). At present, only a few synthetic ammonia plants are using raw materials other than natural gas, naphtha or heavy oil. In some countries where there is a shortage of liquid and gaseous fuels, solid fuels such as coal and lignite are being tried. Also, when low-cost electric power is available, this power can be used to produce electrolytic hydrogen. Ammonia plants at Nangal, India and Aswan Dam, Egypt are using the electrolytic hydrogen to produce ammonia.

The conventional process for ammonia production is based on the technology of two processes for making synthesis gas (mixture of hydrogen and nitrogen). They are steam reforming and partial oxidation. The steam reforming process is used with natural gas and naphtha while partial oxidation is used with heavy oils. In non-conventional processes the solid fuel such as coal is gasified to generate hydrogen and carbon monoxide. The manufacturing details for the above processes are given in Chapter III.

As indicated in Chapter I, the rapid escalation of natural gas price is causing concern in the US ammonia industry at present. At this stage coal appears to be the prospective alternative feedstock. Waitzman (7) presents a technical and economic review of recent projects for making ammonia from coal. Tennessee Valley Authority (TVA), in an effort to develop and demonstrate a method to make ammonia from coal, decided to retrofit a coal gasification plant on to TVA's small (225 Ton/Day) but modern ammonia plant at Muscle Shoals, Alabama. Various studies are being done to run this plant with 60 percent of the feed being synthesis gas from coal, the remainder being synthesis gas from natural gas or at 60 percent capacity using only coal generated synthesis gas (7). Burnett (12) gives the important details of the TVA's ammonia plant retrofitted with 8 Ton per hour coal gasification and gas purification facility. He points out that present investments in large (1000 Tons per day or more) US ammonia plants can be protected by retrofitting these plants with a provision to use coal. It is indicated that coal at 21 dollars per ton will be competitive with natural gas at 3.58 dollars per million BTU. Waitzman et.al (13) discuss coal handling and location of new plants for coal based ammonia plants. It has been mentioned that TVA's ammonia plant is designed to use Illinois No.6 coal as the coal reserves for this coal are greater than any other coal in the United States. In the present study Illinois No.6 coal is also considered and this plant is located in the midwest where most of the fertilizer in the US is

consumed. Waitzman concludes that coal feedstock and fuel represent about 30 percent of the f.o.b price of coal based ammonia. In comparison, the feed and fuel represent around 60 percent for natural gas based ammonia. However, the capital and operating costs associated with the handling and preparation of coal feed are much higher than the costs associated with natural gas feed.

Strelzoff (8) studies the future feedstocks for ammonia production and concludes that the ammonia industry will improve their economics by switching over to coal in the near future as the other feedstocks such as naphtha and natural gas will be much more in demand for other petro-chemicals, thus reducing their availability for ammonia. Netzer and Moe (9) summarize desirable features of the process for coal to ammonia and conclude that the Texaco Coal Gasification Process has all the desirable features and appears to be the promising contender. They also study the economics of coal based ammonia plant and conclude that the breakeven cost for natural gas vs coal based feedstock at 12 percent rate of return will be at a gas price of around 2.6 dollars per million BTU and at a coal price of 85 cents per million BTU. This seems to be questionable at the present time as the ammonia producers still believe that a coal-ammonia process will not be economical even at the present gas price of around 4 dollars per million BTU (15). However, a recent report indicates that a natural gas price of more than 3 dollars per million BTU will have a bad effect on ammonia producers in the US as they can't compete with the imports (11). The present study projects the breakeven point at even a higher natural gas price.

Child (14) mentions the salient features of Texaco coal gasification process. The process advantages claimed for this process are :

1. Texaco process has the capability of operating on virtually all types of coals.

2. It can be operated over wide range of pressures.

3. It has the options for direct quench followed by gas cooling.

Also a split flow combination allows a wide range of steam generation for the steam system to provide down-stream requirements.

4. The raw gas leaving the battery limits doesn't contain phenols, tars and other heavy materials. This minimizes the gas treatment and subsequent environmental problems.

5. The Texaco process is based primarily on coal-water feedstocks which can be readily produced from those normally used in coal slurry pipelines. The Texaco system can be coupled with coal slurry pipelines.

6. The design data required for the Texaco process is readily attainable from Texaco's Montebellow research laboratory and TVA experience.

7. The Texaco process is highly flexible and synthesis gas with few impurities can be produced at elevated pressures.

In the present study the Texaco gasifier is selected to produce synthesis gas, as this process possesses the above cited advantages and has been proven to be effective (there are about 76

licensed plants in 22 countries using Texaco Process). Child (14) mentions that the cost of producing ammonia from coal is sensitive to the method of financing the project, delivered cost of coal and the performance of a particular coal at the gasification conditions. As such, it's desirable that several coals must be evaluated before a sound decision can be reached. Hargreaves and Kirk (15) discuss at length the basis for determining the process parameters and selecting appropriate technology for the production of ammonia from coal. They present a capital cost estimate for a plant producing 1200 Tons of ammonia per day using the Texaco coal gasification process. Their capital cost estimation is high compared to the previous estimates by different authors, but they claim that their estimates are more realistic. They point out that coal conversion of any kind is a capital intensive operation but some relief can be obtained by resorting to different financing methods using lower interest rates. It is mentioned that refinement of design is necessary at present, to achieve significant savings. Rothman and Frank (16) developed an interesting study for setting up off-shore plants for the production of ammonia from natural gas and conclude that tariffs will make imported ammonia cost more. Discussing various implications that will arise with such a type of arrangement, they point out that coal gasification for ammonia production is entirely reasonable, competitive and more attractive.

Even though it has been stated that a new trend toward coal based petrochemical plants has been set by the new Tennessee Eastman plant (17), Reid (10) mentions that the question of using

coal as feedstock to make synthesis gas needs reexamination based upon their experience at Tennessee Eastman. However, Ube Ammonia Industry Co., of Ube City, Japan proposed to construct an ammonia plant with 1650 Tons per day capacity. This plant will be using Texaco gasifiers and is scheduled for completion in 1984 (18).

In this study, the economics of producing ammonia from coal is developed with two different types of depreciation methods and compared with conventional process.

2.2 Advanced System for Process Engineering (ASPEN)

In any chemical process plant, the study of any modifications to an existing process involves lot of time and effort. The factors that are to be taken into account include; equipment and personnel safety, new process conditions, new investment, return on investment and environmental protection. Considerable effort is required to work out all these details by hand. In case of a new plant or development of a new process, various factors are to be studied in depth. This kind of study is to be made with different process conditions and parameters. To evaluate these factors in detail requires many man-hours. However, recent developments in computer-aided design offer rapid, efficient and consistent solutions to these problems. ASPEN is one of the computer-aided design simulators which can be applied easily to any process.

ASPEN, the most recent process simulator, was developed at Massachusetts Institute of Technology in 1979 (32). ASPEN was initially written to provide technical and economic analyses for

the fossil energy conversion processes. It is aimed at identifying problems in various processes, before beginning costly construction of pilot and demonstration fossil fuel plants. Even though ASPEN is developed to aid fossil fuel technology, it is applicable to almost all conventional processes.

ASPEN was developed in close coordination with various industrial companies and government groups and has been tested at various occasions. Gallier et.al (19) present the final version of ASPEN as a system containing 353,482 lines of Fortran code with 1511 individually executable subroutines. Gallier and Evans (20) describe various functions and capabilities of the ASPEN program.

ASPEN can perform steady-state material and energy balances, calculate sizes of equipment and carryout economic evaluations. The main programs that are included in ASPEN are listed as:

1. A process simulator that translates the ASPEN description of a process flow-sheet into a Fortran calling program and execute.
2. A data regression program that is used to determine selected parameters of physical property models from raw or smoothed data. These parameters can be utilized by the process simulator.
3. A program for generating tables of physical properties that are calculated from ASPEN models.
4. A cost estimation and economic evaluation program that can be called directly by the process simulator or on a stand-alone basis to determine capital investment, annual operating costs and various measures of profitability for a simulated process.

The ASPEN process simulator is a powerful system and offers complete flexibility for the simulation of chemical, petroleum, syn-fuels and other industries. It allows the user to perform mass and energy balances around almost all of the unit operations. The various models available are listed in Table 2.1. In addition to these models, the user may choose to estimate his own process models to represent special models called USER MODELS.

The physical property system in ASPEN is supported by a file of data on conventional compounds and contains correlation constants for more than 480 conventional compounds (20). The various properties that can be calculated are, enthalpy, entropy, free energy, molar volume, equilibrium ratio, fugacity coefficient, viscosity, thermal conductivity and diffusion coefficient. The user can specify his own property route or routes depending upon the process conditions prevailing at different sections of the process flow-sheet. There are 12 different physical property options available to choose from.

The cost estimation and economic evaluation system in ASPEN is designed so that it can be used independently to evaluate the size and cost of different equipments or it can be run in conjunction with unit operations simulation, to determine the effects on cost by process decisions. ASPEN contains 17 different process costing models, each with many options. There is a provision to supply the cost indices so that present or future costs can be evaluated. The accuracy of cost estimation by ASPEN will be in the range of ± 30

TABLE 2.1

UNIT OPERATION MODELS AVAILABLE IN ASPEN

1. FLASHES AND HEATERS	5. CRUSHERS AND SCREENS
General purpose heater	
Two outlet stream flash	6. GAS-SOLID SEPARATION
Three outlet stream flash	Fabric filter
Heat exchanger	Cyclone
	Electrostatic precipitator
2. STAGED SEPERATION	
Short cut distillation design	7. LIQUID-SOLID SEPARATION
Short cut distillation rating	Hydrocyclone
Rigorous distillation	Filtering centrifuge
	Rotary vacuum filter
3. REACTORS	
Stoichiometric reactor	8. STREAM MANIPULATORS
Specified yield reactor	Multiplier
Multiphase euilibrium reactor	Duplicator
Continuous stirred tank reactor	Class changer
Plug flow reactor	
	9. GENERAL MIXER
4. PUMPS AND BLOWERS	
Pump/slurry pump	
Single stage compressor/turbine	

percent (20). ASPEN can be further utilized to generate a capital cost estimate, operating costs and profitability analysis for the entire process.

In the present study, ASPEN is used to perform the material and energy balances for different process flow-sheets and obtain the cost of some of the equipment.

2.3 CASHFLOW

CASHFLOW is a Fortran computer program for determining the cost of a product from a production facility, using discounted cash flow procedure. It was originally developed at Oak Ridge National Laboratory as PRP (13) and modified by IEA coal research in London, England. Originally there was a provision to use three different types of depreciation methods. The Chemical Engineering department at University of Tennessee, Knoxville added an additional depreciation method to evaluate the economics using the 1981 US Tax revision depreciation method.

The input data for CASHFLOW are entered by a card format for different items. There is provision to calculate either the price of main product or the rate of return on equity. The principal input data required to evaluate the product cost can be listed as under:

1. Project life, operating life and construction period.
2. Type of depreciation method and depreciable life.
3. Total capital investment.
4. On stream efficiency for each year.
5. Rates of consumption and unit costs of all feedstocks.

6. Rates of production of all products and unit costs of by-products.

7. Tax-rates.

8. Debt-Equity ratio and interest rate on debt.

9. Rate of return on equity.

The different types of depreciation methods available are :

1. Sum of the years digits.

2. Straight line

3. Double declining balance.

4. Tax revision (1981) schedule.

There is a provision to run the program without any depreciation allowances. CASHFLOW offers a wide range of parameters that can be used to determine the discounted cash flow. It has provisions to consider negative federal income taxes, interest during construction, income tax loss carry-forward and different classes of depreciation.

CASHFLOW furnishes details regarding debt repayment data, annual depreciation allowances, outstanding capital investment, working capital, income and cashflow for each year of operation.

In the present study, the product costs of ammonia for widely different cases are developed using CASHFLOW.

CHAPTER III

PROCESS DESCRIPTIONS

As indicated earlier, ammonia is manufactured most often through a natural gas-steam reforming process. The non-conventional process involves gasification of coal. In this chapter, the process details for conventional process (natural gas-ammonia) and non-conventional process are presented.

As mentioned earlier, one of the objectives of the present study is to assess the savings by switching over to alternate fuel supply arrangements in the conventional process. The alternate arrangements considered are an atmospheric fluidized bed combustor and a medium b.t.u gasifier. The process details for these arrangements are also given.

3.1 Technology for the manufacture of Ammonia

3.1.1 Conventional process: Natural gas--Ammonia

The block diagram in Figure 3.1 shows the principal stages for manufacturing ammonia. Strelzoff (6) has dealt extensively with the manufacturing details of ammonia production.

In general, the processing steps involved in the manufacture of ammonia are:

1. Feed desulfurization
2. Primary reforming
3. Secondary reforming
4. Shift conversion

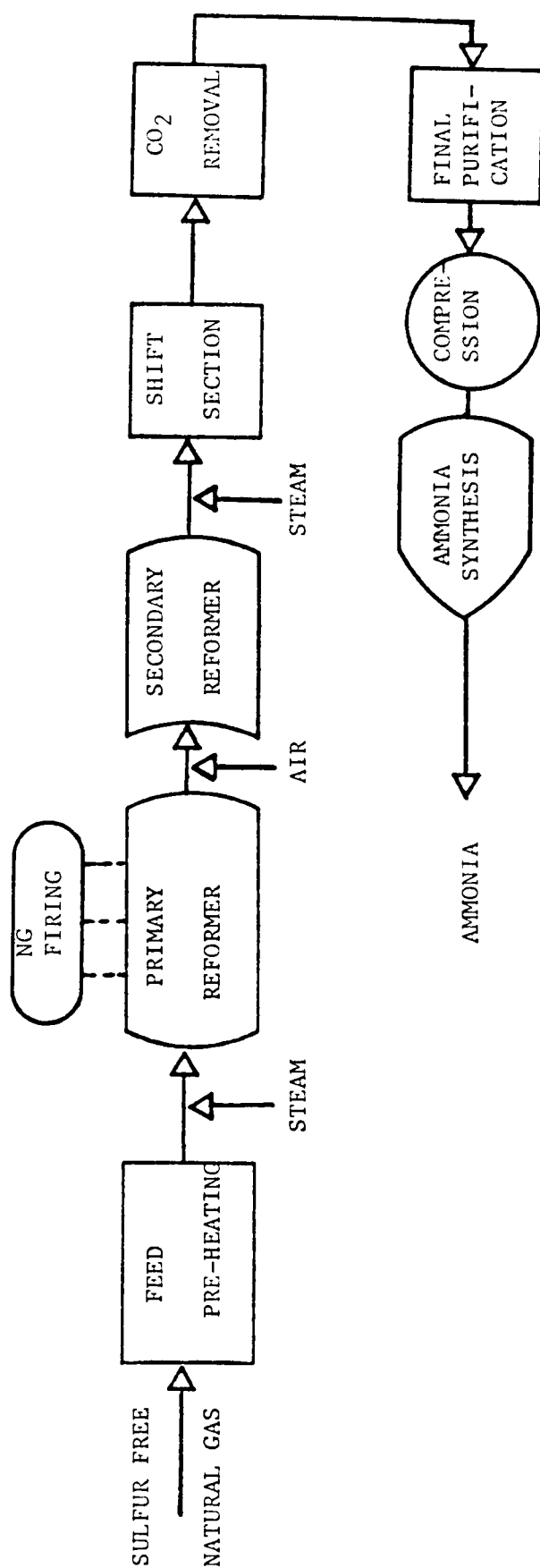
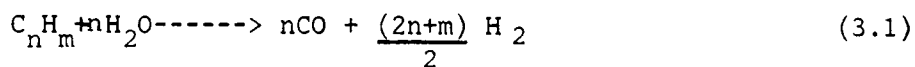


Figure 3.1. Block diagram for manufacturing ammonia by conventional process with natural gas as raw material

5. Carbon-dioxide removal
6. Methanation
7. Synthesis gas compression
8. Ammonia synthesis and condensation
9. Inert gas purge
10. Ammonia refrigeration

The feed natural gas is preheated to about 750 deg F and passed through desulfurizers, to decrease the sulfur content in the gas to about 0.2 ppm. Zinc oxides are utilized for the desulfurization. The desulfurized gas is then mixed with process steam and sent to reforming section.

In general, the reaction of steam and a hydrocarbon to produce synthesis gas containing CO and H₂ can be represented by



When methane (natural gas) is used as the feed stock, the above reaction can be simplified to



The methane/steam reaction is highly endothermic to the extent of requiring 97,300 BTU/lb-mole. The above reaction to produce synthesis gas is favoured by three factors. These factors are low pressure, high temperature and high steam/carbon ratios. In recent years, reforming has been performed at high pressures for the following reasons:

1. Natural gas which is generally available at high pressures can be utilized directly without reducing the pressure.
2. Better heat recovery from the condensate is possible at the higher pressure levels.

3. Smaller size equipment and piping can be used.
4. The water gas shift converter is more efficient at higher pressure allowing smaller pieces of equipment and less catalyst.
5. The carbon dioxide removal system is more efficient and compact.

Typically, most of the primary reformers are operated over a pressure range of 450-500 psig and a temperature range of 1600-1700 deg F. The feedstock generally enters the catalyst-filled tubes at a temperature of 850-1050 deg F. It is important that steady state conditions be maintained as far as possible in the reformer to avoid thermal cycling of the tubes. The heat required for the endothermic reaction is supplied by burning natural gas as fuel. The conventional heat flux will be around 20,000 BTU/sq.ft-hr (6). The hot flue gas will be used in several heat recovery systems: a feed preheat coil, process air preheat coil and combustion air preheater before exiting the stack.

Roof-fired box and Terrace-wall type designs are utilized for the conventional type reformer furnaces (6). In roof fired furnaces as the name implies, the burners will be firing down from the roof, between tube rows. The flue gas leaves the firebox through the ducts arranged in the furnace bottom. Different kinds of fuels can be used in this type of furnace; however the burners are less accessible. It is difficult to adjust the heat flux along the length of the tube, which ultimately may result to form carbon in the upper part of the tubes. Recent developments however, offer a more uniform temperature profile. Terrace wall furnaces offer relatively good control of heat flux along the length of the

catalyst tube. There will be no impingement of flame and there is a wide choice of fuels for this furnace. In the terrace wall furnace, the inclined terrace walls are heated by burners fired from both sides, at multi levels. Kraus (26) describes various process implications involved in the design of reformer furnaces.

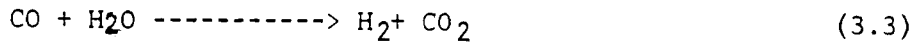
The burners in a reforming furnace must distribute the flames and nascent combustion products uniformly across the reradiating refractory walls of the furnace. Currently, there are three different types of burners (6). They are, air inducting type for liquid fuels, non-air inspirating type for gaseous fuels and combination burners having provision for both oil and gas.

Various kinds of reformer catalysts are presently available with various trade names. Calcium-aluminate-silicate and nickel based catalysts are commonly used (6). These catalysts will have a service life of about four years. Sulfur and arsenic are the common catalyst poisons. Bridger (25) presents various desirable features of reforming catalysts.

In the secondary reformer, the conversion of methane to hydrogen and carbon oxides is substantially completed. The exit gas from the primary reformer along with pre-heated air is supplied as the feed to secondary reformer. This is operated at a temperature of about 1830 deg F and nickel with high alumina is used as a catalyst (6).

The process gas leaving the secondary reformer is cooled to about 675 deg F by passing it through the process steam generator

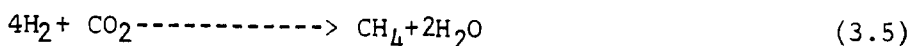
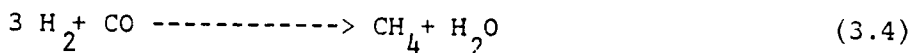
and feed gas pre-heater. The carbon monoxide will be converted into additional hydrogen by the catalytic water-gas shift reaction:



Because a single stage shift reactor requires very large amounts of steam which is not economical, the above reaction is carried out in two or more stages, allowing about 70 percent conversion in first stage. The overall conversion is around 97 percent. Iron-Chromium catalyst is used in the first stage (high temperature shift) and Copper-Zinc catalyst is used in the other stages (low temperature shift).

Carbon-dioxide in the stream from shift converter is generally removed either by water scrubbing or monoethanolamine (MEA) absorption. Absorption with hot potassium carbonate is also widely used (6). In the MEA absorption process, product gas at around 150 deg F flows to the absorber and is contacted with 30 percent (by weight) MEA solution. Regeneration will be accomplished by pressure release and reboiling the solvent solution. The carbon-dioxide removed will be around 1.22 tons per ton of ammonia. Generally this is vented to atmosphere.

The carbon oxides left in the process gas leaving the carbon dioxide removal system are converted to methane in Methanator by the following reactions:



These reactions are exothermic and take place over a nickel catalyst. The purified feed gas is compressed and mixed with

recycle gas from synthesis reactor. The gas mixture is compressed to about 300 atmospheres. The combined feed is cooled to condense recycled ammonia and water after which they are separated. The compressed gas is then heated in a feed-effluent heat exchanger and fed to the synthesis reactor. Ammonia forms in the reactor as per the reaction



The most economical synthesis pressure is around 4500 psig. The converter effluent is cooled to around 175 deg F. This heat is utilized to generate steam. The synthesis catalysts generally employed are based on metallic iron promoted with alkali metals such as potassium, alumina and magnesia (6). The inerts from synthesis loop are removed by purging a part of the recycle.

The ammonia refrigeration system consists of a closed loop ammonia circulation. The ammonia vapors are condensed in the system and product ammonia is withdrawn at about 22 deg F.

3.1.2 Non-Conventional Process: Coal--Ammonia

The process route showing the important steps in the manufacture of ammonia from coal is given in Figure 3.2. Various process steps involved in the above process can be summarized as:

1. Coal preparation
2. Slurry preparation
3. Air separation
4. Coal gasification
5. Shift conversion

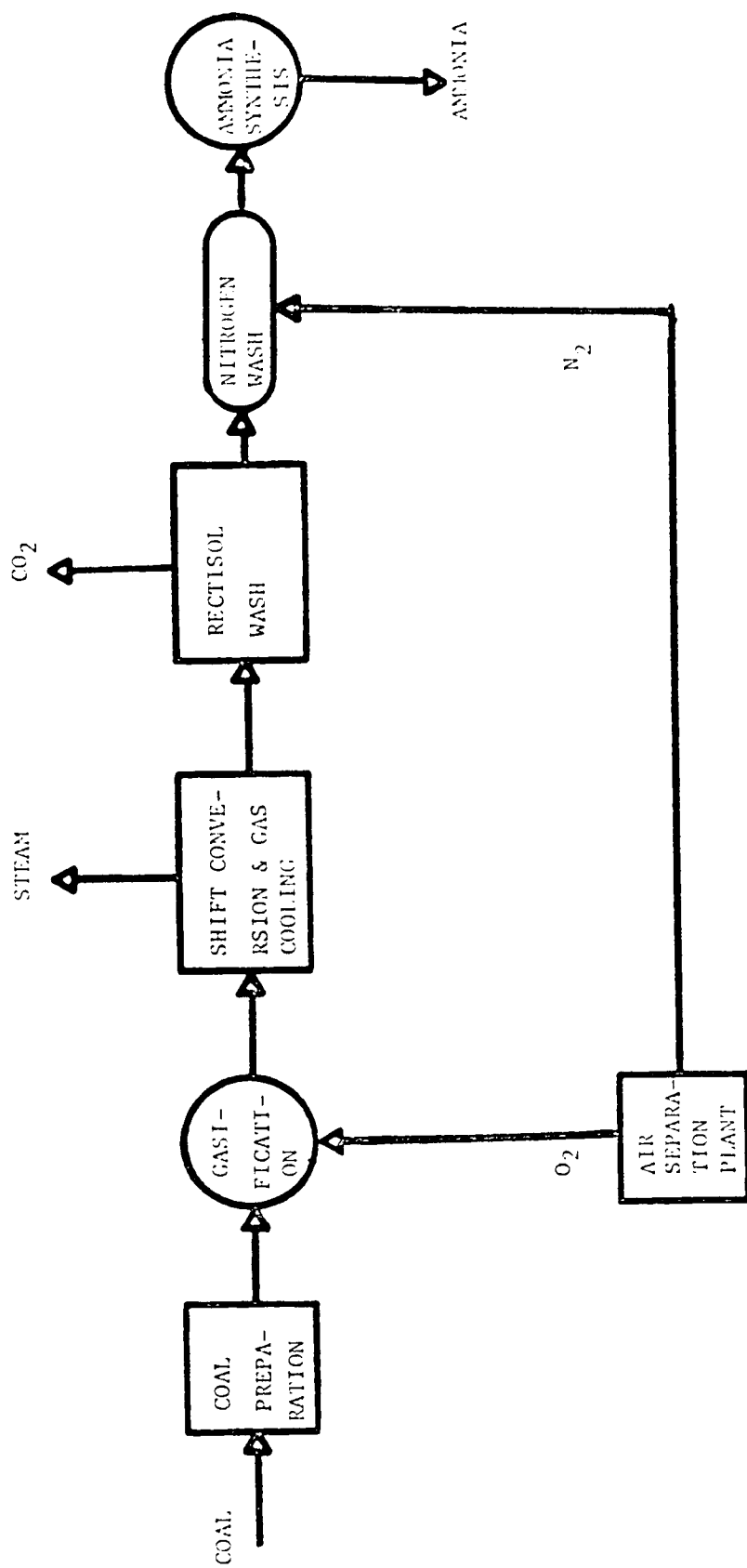


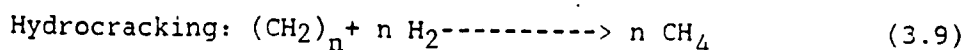
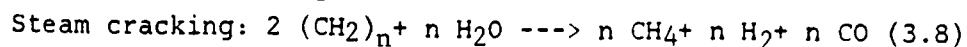
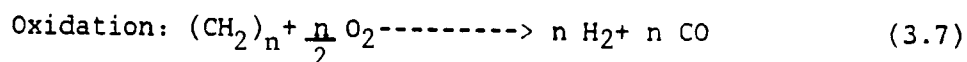
Figure 3.2. Flow diagram for ammonia manufacture by non-conventional process with coal as raw material

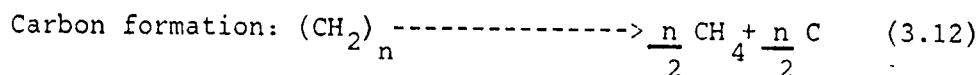
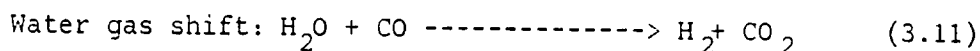
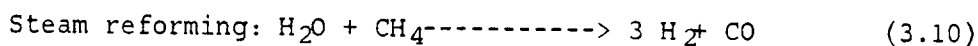
6. Acid gas separation
7. Liquid nitrogen wash
8. Ammonia synthesis

Coal is unloaded from rail cars and crushed to pass a 3/4 inch screen. Crushed coal is stored in live and dead stockpiles and fed to slurry preparation unit.

In the present process, coal is gasified by Texaco coal gasification process. The distinctive feature of this process is the feeding of coal to gasifier in the form of coal-water slurry. Coal from the coal preparation area is ground in a wet grinding mill and slurried with water. This slurry consists of solids to an extent of 55 percent by weight.

The slurry is pumped from a slurry hold tank to a burner, located in the head of the gasifier. Oxygen of nearly 99.5 percent purity is also supplied to the burner. The reactants enter the gasifier which operates at about 60 atmospheres pressure and react exothermally to produce a gas containing mainly of carbon monoxide, hydrogen and carbon-dioxide together with unconverted water. Sulfur compounds in the coal are also gasified in the reactor to produce primarily hydrogen sulfide and carbonyl sulfide. Small quantities of other compounds such as ammonia and methane are also formed. Some of the typical reactions occurring in the gasifier can be represented as:



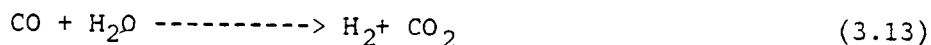


The gasification temperature is higher than the ash fusion temperature of feed material so that no tars, phenols or other undesirable by-products are produced. To withstand the severe reducing environment, the top section of the gasifier is lined with a special type of refractory material. To limit the temperature to which the refractory material can withstand, a moderator (usually water in feed) is also added. The lower section of the gasifier is a quench chamber where the gasification products are rapidly cooled by contact with water. During this process, the slag solidifies and the gas is saturated with water vapor. The slag is withdrawn from the gasifier by a lock hopper arrangement.

The Texaco process can be operated in two different modes:

1).Direct quench with internal steam generation and 2).Gas cooler with external steam generation. In the case of synthesis gas generation for ammonia production the direct quench mode is used.

The effluent gas leaving the gasification area is fed to catalytic shift converters. Additional hydrogen is produced in these reactors by the water-gas shift reaction:



This reaction is carried out in two stages with a cooling arrangement for the gas between the stages. The gas leaving secondary stage shift reactor contains around 2 percent carbon monoxide.

Sulfur compounds and carbon-dioxide are removed from shifted gas by the Rectisol process. The gas is cooled to very low temperatures (-20 degree F) and scrubbed with methanol. This reduces the concentration of sulfur compounds (mainly hydrogen sulfide and carbonyl sulfide) to about 1 ppm and carbon dioxide to 30 ppm. Hydrogen sulfide is selectively concentrated to about 35 percent and sent to the sulfur plant. In the sulfur plant, hydrogen sulfide is converted to elemental sulfur.

Molecular sieves are used to remove traces of carbon-dioxide and methanol from treated gas leaving the methanol wash column. This gas is further scrubbed with liquid nitrogen to remove any carbon monoxide, methane and argon left in the gas. The overhead gas from nitrogen wash scrubbing tower contains less than 5 ppm of carbon monoxide.

Nitrogen from the air separation plant is added to the product gas to produce an H_2 : N_2 ratio of 3:1. This gas mixture is compressed to about 300 atmospheres and sent to synthesis reactors. The synthesis reactor units are similar to the units in conventional process. The synthesis gas reacts in the presence of a catalyst to form ammonia as per



Ammonia vapors are condensed by water cooling and refrigeration. The liquid ammonia is pumped to storage.

3.2 Combustion and Gasification of Coal

As discussed earlier, coal is considered as a potential supplier of fuel also for the primary reformer in the conventional process. Prior attempts have been made to replace natural gas as fuel in ammonia plants. Demarest (30) has presented details of trials where various oils are burned in the primary reformer furnace replacing natural gas firing. The problems encountered by this operation are plugging of burners, spalling of refractories, soot formation and oil pump failures. It has been stated that switching over to fuel oil system isn't simple and may result major operating problems. Johnson (31) proposes a new system called, VFO (Vaporized Fuel Oil system) to burn oil as well as gas in the same burners. It is claimed that operating costs are lower for this new system, compared to gas burning.

In the present study, coal combustion in an atmospheric fluidized bed combustor and medium btu gas from a Babcock and Wilcox gasifier are considered as two different alternative suppliers of heat energy in the primary reformer. The concept of using coal for a process heater is not new. Barnett et.al (27) present details on how medium btu gas (MBG) can be used for a process heater. Cherrington and Golan (28) discuss various aspects for utilizing fluidized bed coal firing for process heaters. O'Sullivan et.al (29) give details for the design parameters of coal fired process heaters, for various process requirements. McKenzie (59) describes the salient features of coal fired fluidized bed combustors. A brief description of Babcock and Wilcox gasifier and atmospheric fluidized bed combustor is given in the next page.

3.2.1 Babcock and Wilcox gasifier

This is an entrained flow, single stage, two-zone gasifier. Pulverized coal, oxygen and steam are injected through two or more rows of nozzels near the bottom of the lower zone. In this lower zone, coal and recycled char are contacted with oxygen to form synthesis gas. In the upper zone of the gasifier product gas is cooled to between 1600-1800 deg F. Because of the high temperature, the product gas is free from trouble-some tars and phenols. Since gasification is incomplete, this system has a char recycle loop that increases the carbon utilization to more than 98 percent. The product gas will have a heating value of about 300 BTU per cu.ft. Centrifugal forces cause the molten slag formed in the lower zone to impinge on the refractory walls. The molten slag is continuously withdrawn from the base into a quench tank. Char and carbon are separated from the product gas using cyclones and reinjected into the gasification zone.

3.2.2 Atmospheric Fluidized Bed Combustor

The bed material limestone and fuel coal are crushed to a size such that the loss by elutriation is minimum for the chosen fluidization velocity. The bed is fluidized by blowing evenly distributed air through it. The coal is burned with air at velocities sufficient to maintain fluidized bed conditions. The heat absorption surface is immersed in the bed. The process fluid is heated as it flows through the tubes in the fluidized bed. The main advantages for this type of system are:

1. Very high heat transfer coefficients are obtained between the

bed material and immersed surface. Consequently, the overall heat flux will be high even though the temperature differential is low.

2. Because combustion is carried at a relatively low temperature, the coal ash particles are kept below their softening temperature which prevents slagging.

3. There is relatively little variation in the heat flux over all the immersed surface; so there is small risk of tube failure due to high local heat flux.

4. There is potential improvement in overall energy efficiency due to increased combustion efficiency.

5. Low combustion temperature leads to relatively low vapor pressures of alkali metal sulfates and chlorides. Due to this, these harmful constituents remain in the bed.

In the present study, to meet the SO_2 emission standards a dry limestone scrubbing process is used. The dry limestone is added to the pulverized coal. The sulfur oxides formed in the hot bed react with limestone to form calcium sulfate, which is removed along with the ash left from the combustion process. This process requires a mass ratio of limestone to coal of about 1:4 to remove 90 percent of the sulfur oxides.

CHAPTER IV

ASPEN SIMULATION OF AMMONIA AND COMBUSTION PROCESSES

As indicated earlier, ASPEN is used to perform material and energy balances for different processes in this study. To simulate a flowsheet by ASPEN, various stages are to be modeled with different unit operation blocks available in ASPEN. The required process conditions and parameters are also to be supplied. ASPEN input language mainly consists of three different key words namely, primary, secondary and tertiary. All the paragraphs start with primary key words and all sentences start with secondary key words. Tertiary key words are generally used for the data entry. A line in ASPEN can contain a maximum of 80 characters however, there is no limit on number of lines. A sentence can be continued on as many additional lines as necessary, if entries are not split, by terminating each line with an ampersand character and leaving at least the first column blank on each additional line. There are three different options for units, SI, English and Metric. The default option is English units. There are numerous number of other rules for ASPEN input language. A detailed description of these rules can be found in ASPEN user manual under syntax and global data section (34). The ASPEN code used to simulate various flow-sheets and the ASPEN output results for the simulated processes are presented in this chapter. The capacity of the ammonia plant in this study is fixed at 1000 tons (short) of ammonia per day. This capacity is selected as it is reported that optimum operating costs appear close to that capacity (35).

4.1 Natural gas--Ammonia

The conventional process for manufacturing ammonia from natural gas is simulated with ASPEN. Various stages in the process are modeled with reactors, heaters, splitters etc. For convenience, the flow-sheet is divided so that material balances and steam and energy balances can be performed separately.

4.1.1 Material balances

The principal manufacturing stages shown earlier in Figure 3.1 are modeled with ASPEN unit operation blocks. Figure 4.1 shows the flow scheme of the conventional process simulated by ASPEN.

The raw material for the present process is natural gas. As there is no single compound in ASPEN data bank to represent natural gas alone, various constituents of natural gas are represented by different compounds as per the composition. All these compounds are mixed to represent the natural gas. Typical composition of natural gas considered in the present study is given in Table 4.1. In this composition, hydrogen sulfide, carbon dioxide and some hydrocarbons which are present in very low amounts are not represented for the reasons of simplicity. Also, a desulfurization step is not included in the present flow-sheet.

The present process involves high pressures and temperatures. As such, the ASPEN physical properties option set SYSOP 4 is selected. This set covers a wide range of pressures and temperatures. The ASPEN input code required for obtaining physical

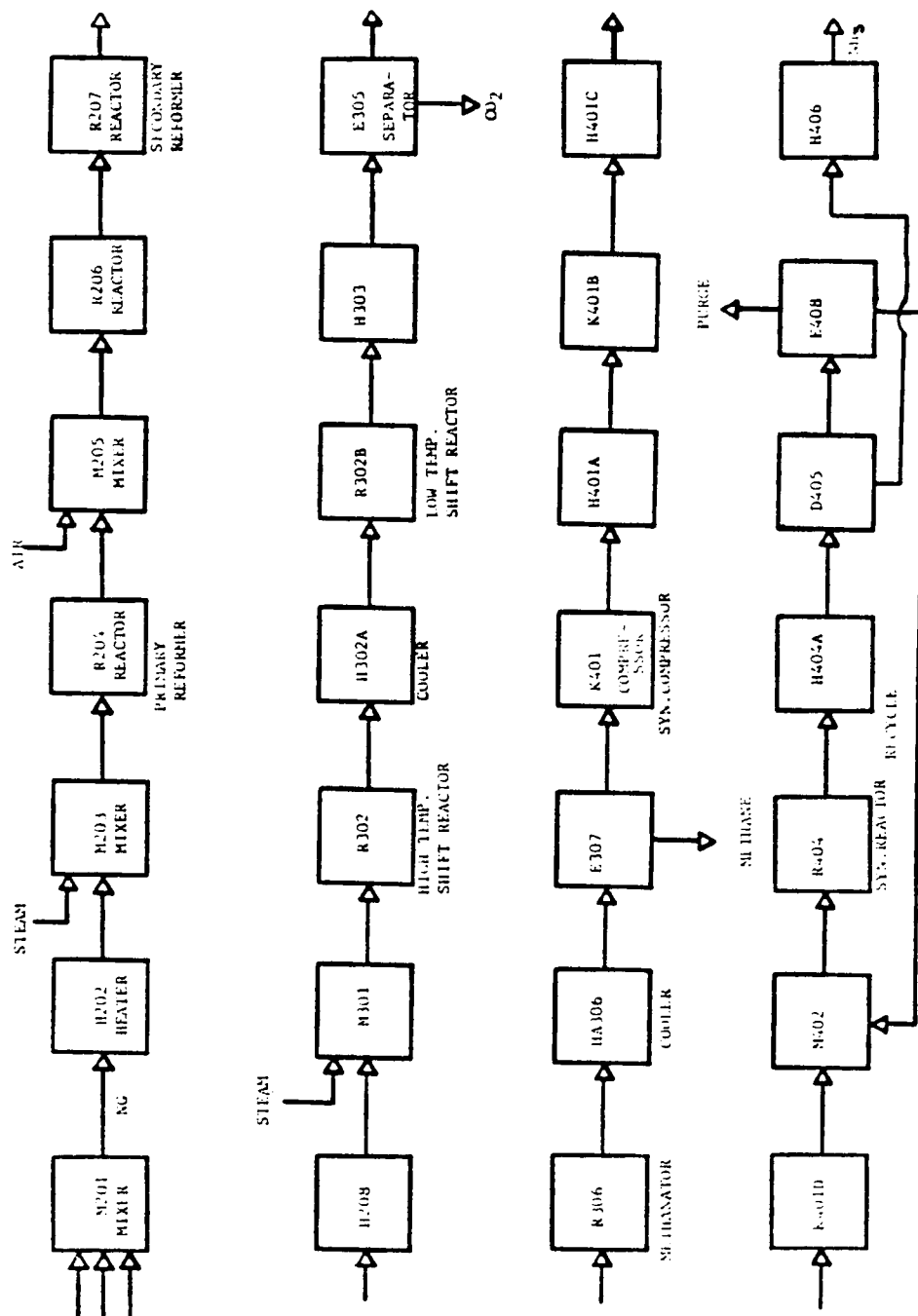


Figure 4.1. Flow scheme for ASPEN simulation - Conventional process for manufacturing ammonia from natural gas

TABLE 4.1
TYPICAL COMPOSITION OF NATURAL GAS

Component	Percent by volume
Methane	93.25
Ethane	3.30
Propane	1.09
Nitrogen	1.95
Argon	0.40

Source: Strelzoff, S, Technology and Manufacture of Ammonia, John Wiley and Sons Inc, New York, 1981, p. 104.

property data is presented in Figure 4.2. The input data for various process streams are supplied in metric units and it's code is also shown in Figure 4.2.

In ASPEN all the unit operations blocks will be connected by streams. The raw material is supplied through input streams to the first block in most of the cases. The output stream of the previous block becomes the input stream to the succeeding block or in other words, the streams establish a connectivity between the blocks. For the present flow sheet for the conventional process, the entire flow sheet is divided into three different sections. They are the reforming, shift and synthesis sections. The stream representation is given by starting the stream name with the letter S (example S201, S202 etc.). The connectivity of the unit operation blocks with various streams for the present flow sheet is shown in Figure 4.3.

As indicated earlier, the main raw material (natural gas) is formed by mixing various constituents of the natural gas. Block M201 is used as a mixer to mix all the five input streams. The input stream details for the natural gas necessary to produce 1000 tons of ammonia per day is given in Table 4.2. It is observed that a total feed gas of 740,645 scf/hr is required. The total natural gas requirement (feed + fuel) is calculated in the later part of this chapter after assessing the heat load of the primary reformer.

The feed stream is preheated by a heater block H202. The process steam required for the steam reforming reaction is supplied through S208, with a flow rate of 30,088 kg/hr. The primary

```

IN-UNITS  MET  TEMPERATURE=C
OUT-UNITS  MET  TEMPERATURE=C
;
;*****
;          PHYSICAL PROPERTY DATA
;*****
;
COMPONENTS  AR AR / C2H6 C2H6 / H2 H2 / CO CO / CO2 CO2 / N2 N2 /
            O2 O2 / H2O H2O / H3N H3N / CH4 CH4 / C3H8 C3H8
PROPERTIES  SYSOP4 GLOBAL
;
;
COMP-NAMES  AR ARGON / C2H6 ETHANE / H2 HYDROGEN / CO CARBONMONOXIDE /
            CO2 CARBONDIOXIDE / N2 NITROGEN / O2 OXYGEN / H2O WATER /
            H3N AMMONIA / CH4 METHANE / C3H8 PROPANE
;

```

Figure 4.2. ASPEN Code for physical property data

```

;
FLOWSHEET
;
;REFORMING SECTION
  BLOCK M201          IN=S201  S202 S203 S204 S205          OUT=S206
  BLOCK H202          IN=S206                                OUT=S207
  BLOCK M203          IN=S207  S208                          OUT=S209
  BLOCK R204          IN=S209                                OUT=S210
  BLOCK M205          IN=S210  S211 S218                      OUT=S212
  BLOCK R206          IN=S212                                OUT=S213
  BLOCK R207          IN=S213                                OUT=S214
  BLOCK H208          IN=S214                                OUT=S215
;
;SHIFT SECTION
  BLOCK M301          IN=S215  S301                          OUT=S302
  BLOCK R302          IN=S302                                OUT=S303
  BLOCK H302A         IN=S303                                OUT=S304
  BLOCK R302B         IN=S304                                OUT=S304A
  BLOCK H303          IN=S304A                              OUT=S305
  BLOCK E305          IN=S305                                OUT=S308  S309
  BLOCK R306          IN=S308                                OUT=S310  SA310
  BLOCK HA306         IN=S310                                OUT=S311
  BLOCK E307          IN=S311                                OUT=S312  S313
;
;
;SYNTHESIS SECTION
  BLOCK K401          IN=S312                                OUT=S312A
  BLOCK H401A         IN=S312A                              OUT=S401A
  BLOCK K401B         IN=S401A                              OUT=S401B
  BLOCK H401C         IN=S401B                              OUT=S401C
  BLOCK K401D         IN=S401C                              OUT=S401
  BLOCK M402          IN=S401  S411                          OUT=S403
  BLOCK R404          IN=S403                                OUT=S404
  BLOCK H404A         IN=S404                                OUT=S405
  BLOCK D405          IN=S405                                OUT=S406  S407
  BLOCK H406          IN=S406                                OUT=S408  Q1
  BLOCK E408          IN=S407                                OUT=S411  S412

```

Figure 4.3. Connectivity of streams with various blocks in conventional process flow sheet

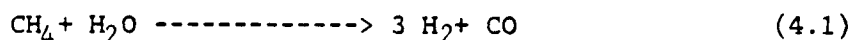
TABLE 4.2

STREAM DETAILS FOR REPRESENTING NATURAL GAS

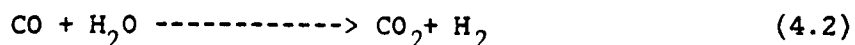
Stream	Constituent	Flow rate: k-mole/hr
S201	Methane	872.86
S202	Ethane	30.88
S203	Propane	10.21
S204	Nitrogen	18.09
S205	Argon	3.71
S206	Natural gas	935.75 (740,645 scf/hr)

reformer is modeled with a stoichiometric reactor. The ASPEN code for the primary reformer is given in Figure 4.4 which includes the stoichiometric equations for the various reactions. The operating temperature, pressure and the corresponding methane conversion are selected as per the literature (6). The composition of the effluent stream from the reformer (S210) can be seen in Appendix A-II in which the stream data obtained from ASPEN simulation for various streams are presented. The steam reforming reaction is highly endothermic. The heat required for this reaction and the total heat load for the primary reformer furnace is evaluated with another ASPEN run and will be presented in the energy balance section, later in this chapter.

Nitrogen required for the synthesis is mixed (in the form of air) with the primary reformer effluent stream and sent to the secondary reformer. The total air flow is 1198 k-moles per hour. In the secondary reformer the conversion of methane is substantially completed. The secondary reformer is modeled as another stoichiometric reactor R207, where the reaction



takes place. Some of the natural gas is burnt with oxygen (present in the air) to supply the necessary heat. These reactions are carried out in another reactor R206. The product gas is cooled and sent to shift section. The steam required for shift reactor is mixed in a mixer M301. The steam requirement for the shift reactor is 14,555 kg per hour. The shift reaction



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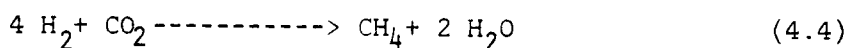
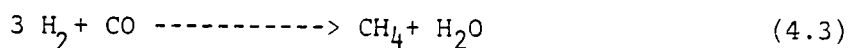
;THE REACTIONS ASSUMED TO OCCUR IN THE PRIMARY REFORMER ARE
;  CH4+H2O----> CO+3H2;    C2H6+4H2O---->7H2+2CO2
;  C3H8+6H2O----->10H2+3CO2
BLOCK  R204  RSTOIC
      PARAM  TEMP=770  PRES=16  NPK=1
      STOI  1  MIXED CH4  -1 / H2O  -1 / CO  1 / H2  3
      STOI  2  MIXED C2H6  -1 / H2O  -4 / H2  7 / CO2  2
      STOI  3  MIXED C3H8  -1 / H2O  -6 / H2  10 / CO2  3
      CONV  1  MIXED CH4  0.60
      CONV  2  MIXED C2H6 0.95
      CONV  3  MIXED C3H8 0.95

```

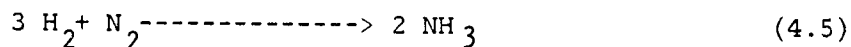
Figure 4.4. ASPEN code for primary reformer-- Conventional process

is carried out in two stages represented by two stoichiometric reactors R302 and R302B. The operating conditions are chosen as per the literature (6).

After cooling the shifted products, the product gas is sent for carbon dioxide removal. In the present flowsheet, carbon dioxide removal is achieved through a separator E305. The desired fractional separations for all the constituents are to be supplied as input data for this unit operation block. The final purification of synthesis gas is done in a methanator, modeled as an equilibrium reactor R306 to carry out the reactions:



The ASPEN code for the carbon dioxide separation and the methanator is given in Figure 4.5. The process conditions for the methanator are as per the literature (36). The removal of methane from the syn-gas is done through another separator E307, which simulates a final purification, before the gas is compressed to high pressures. The three stage compression of the syn-gas is represented by blocks K401, K401B and K401D. The synthesis reactor is considered as a stoichiometric reactor R404 in which the reaction



takes place. The reaction conditions and the corresponding conversion are taken as per the literature (6). In the synthesis loop, some of the recycle is purged to avoid the inerts build up. The unit operation block E408 which represents a splitter is used to purge some of the recycle. Heater block H406 is used to cool

```

BLOCK  E305    SEP2
; THIS IS TO REMOVE CARBONDIOXIDE BY MEA PROCESS.IT IS ASSUMED THAT
; 99% OF CO2 IS REMOVED BY THIS PROCESS.
  FLASH-SPECS  S308  TEMP=300  PRES=21  NPK=1  KPH=1/
                  S309  TEMP=65    PRES=21  NPK=1  KPH=1
  FRAC SUBS=MIXED STRM=S308 COMP=H2 CH4 CO CO2 N2 O2 C3H8 H2O C2H6 AR &
    FRAC=.999 .999 .999 .01 .999 .999 .999 .999 .999 .999 /
    STRM=S309 COMP=H2 CH4 CO CO2 N2 O2 C3H8 H2O C2H6 AR &
    FRAC=.001 .001 .001 .99 .001 .001 .001 .001 .001 .001
BLOCK  R306    REQUIL
;
; THIS IS METHANATOR FOR FINAL PURIFICATION OF SYNTHESIS GAS
;THE REACTIONS INVOLVED ARE 3H2+CO--->CH4+H2O ; 4H2+CO2--->CH4+2H2O
  PARAM NR=2    TEMP=310  PRES=21  NPK=1
  STOI  1  H2  -3 0 / CO  -1 0 / CH4  1 0 / H2O  1 0
  STOI  2  H2  -4 0 / CO2 -1 0 / CH4  1 0 / H2O  2 0

```

Figure 4.5. ASPEN code for carbon dioxide removal and methanator in conventional process

ammonia vapors coming from the synthesis reactor. The product stream coming from the block H406 will be sent to ammonia storage.

The main inputs and outputs for this process flow sheet are presented in Table 4.3. The ASPEN code used to simulate the entire flow sheet is given in Appendix A-I. The stream data for various streams are presented in Appendix A-II.

4.1.2 Steam and Energy balances

As indicated earlier, one of the objectives of the present study is to assess the savings by switching over to alternative fuels for the primary reformer furnace. In order to evaluate the alternative fuel consumption and to size the new arrangement, the heat load for the furnace is to be evaluated. ASPEN is used to perform the heat balances and to evaluate the heat load of the furnace.

In general, the primary reformer furnace in a conventional process supplies heat to the following:

1. Feed pre-heating coil
2. Air(for secondary reformer) heating coil
3. Endothermic heat for steam reforming reaction
4. Boiler feed water heater
5. Steam generation coil
6. Steam superheating coils

In this study, the above heat loads are assessed with the help of ASPEN and added up to arrive at the total heat load of the furnace.

TABLE 4.3

MAIN INPUT AND OUTPUT STREAMS--CONVENTIONAL PROCESS

Input	Output	Stream	Flowrate
stream ID	stream ID		
S206		Gas feed	740,645 scf/hr
S208		Steam for reformer	66,316 lb/hr
S211		Nitrogen for synthesis	2,552 lb-mole/hr
S301		Steam for shift reactor	32,080 lb/hr
	S408	Ammonia product	1,004 tons/day

As mentioned earlier, the pre-heating of feed is carried in a heater represented by a block H202 (see Figures 4.1, 4.3 and Appendix A-I). From the ASPEN simulation results it is found that the heat load required to raise the temperature of the feed to 752 degree F is 11.54 million BTU per hour. The ASPEN results for the above are shown in Figure 4.6.

A separate ASPEN program is simulated to calculate the heat load for air heating coil. In this, the unit operation blocks Mixer, Compressor and Heater are used to simulate a flow sheet in which nitrogen and oxygen at atmospheric pressure and temperature are mixed, compressed to a pressure of 345.5 psi and heated to a temperature of 950 degree F. From the ASPEN results the heat load for the heater is observed to be 14.13 million Btu per hour.

The endothermic heat of reaction is evaluated with another ASPEN run. The natural gas and steam flow rates are considered as per the previous ASPEN code (see Appendix A-I) used for the process simulation of the conventional flow sheet. The primary reformer is modeled as a stoichiometric reactor. The overall conversion of methane, ethane and propane is assumed to be 87.5 percent. As indicated earlier, the steam reforming process is actually carried in two stages (primary and secondary). However, in estimating the endothermic heat in the present case, the reaction is assumed to occur in one reactor. The heat load from the ASPEN results is observed to be 232 million BTU per hour. The ASPEN code and the results obtained for the reactor are presented in Figure 4.7.

GENERAL-HEAT (HEATER): H202
 FEED PRE-HEATER
 INPUT STREAM: S206
 OUTPUT STREAM: S207
 PROPERTY OPTION SET SYSOP4

*** INPUT DATA ***	
TWO PHASE TP FLASH	
SPECIFIED TEMPERATURE C	400.00
PRESSURE DROP ATM	-1.0000
MAXIMUM ITERATION NO.	30
CONVERGENCE TOLERANCE	.100000D-03
TP FLASH, NO INITIAL GUESSES ARE REQUIRED	

*** RESULTS ***	
OUTPUT TEMPERATURE C	400.00
OUTPUT PRESSURE ATM	31.000
HEAT DUTY CAL/SEC	.80723D+06
VAPOR FRACTION	1.00000

Figure 4.6. ASPEN results for feed pre-heater heat load--Conventional process

BLOCK R204 RSTOIC

PARAM TEMP=770 PRES=16 NPK=1

STOI 1 MIXED CH4 -1 / H2O -1 / CO 1 / H2 3

STOI 2 MIXED C2H6 -1 / H2O -4 / H2 7 / CO2 2

STOI 3 MIXED C3H8 -1 / H2O -6 / H2 10 / CO2 3

CONV 1 MIXED CH4 0.875

CONV 2 MIXED C2H6 0.875

CONV 3 MIXED C3H8 0.875

*** RESULTS ***

STOICHIOMETRIC MATRIX:

REACTION # 1:

SUBSTREAM MIXED :

H2	CO	H2O	CH4
3.0000	1.0000	-1.0000	-1.0000

REACTION # 2:

SUBSTREAM MIXED :

C2H6	H2	CO2	H2O
-1.0000	7.0000	2.0000	-4.0000

REACTION # 3:

SUBSTREAM MIXED :

H2	CO2	H2O	C3H8
10.000	3.0000	-6.0000	-1.0000

REACTION CONVERSION SPECS: NUMBER= 3

REACTION # 1:

SUBSTREAM:MIXED KEY COMP:CH4 CONV FRAC: .8750

REACTION # 2:

SUBSTREAM:MIXED KEY COMP:C2H6 CONV FRAC: .8750

REACTION # 3:

SUBSTREAM:MIXED KEY COMP:C3H8 CONV FRAC: .8750

REACTION EXTENT SPECS: NUMBER= 0

ONE PHASE TP FLASH SPECIFIED PHASE IS VAPOR

SPECIFIED TEMPERATURE C 770.00

SPECIFIED PRESSURE ATM 16.000

MAXIMUM ITERATION NO. 30

CONVERGENCE TOLERANCE .10000D-03

TP FLASH, NO INITIAL GUESSES ARE REQUIRED.

*** RESULTS ***

OUTPUT TEMPERATURE C 770.00

OUTPUT PRESSURE ATM 16.000

HEAT DUTY CAL/SEC .16235D+08

Figure 4.7. ASPEN code and results for evaluating endothermic heat in reforming--Conventional process

The steam balance for the conventional process is performed using ASPEN. As indicated earlier (see Table 4.3) the process steam requirements for producing 1000 tons of ammonia per day are 66,316 lb/hr for the primary reformer and 32,080 lb/hr for the shift reactor. In the present process it is considered that high pressure steam at 1500 psi pressure and 900 degree F (superheated steam) will be produced in the reformer furnace. This high pressure steam passes through a main turbine, which drives the syn-gas compressors. A bleed stream from the turbine is taken at 566 psi and 480 degree F (saturated steam). A portion of this steam is utilized as process steam for the reformer. The remaining is superheated to 750 degree F and passed through another turbine. This turbine generates the electric power for miscellaneous purposes. The bleed stream from this turbine provides the process steam for the shift section.

The ASPEN flow sheet for the above is given in Figure 4.8. The heater blocks H101 and H105 represent the boiler feed water heater and steam coil respectively. Superheating of steam is achieved through another heater block H200. The blocks F201 and F203 represent the automatic extraction turbines. The bleed streams from these blocks are the process steam streams.

The ASPEN code to simulate the above flow sheet is presented in Appendix A-III. Special property option SYSOP12 is selected to have the steam properties as per the 1967 ASME (American Society of Mechanical Engineers) steam table correlations. The boiler feed water requirement is observed to be 11,970 lb per hour. A separate

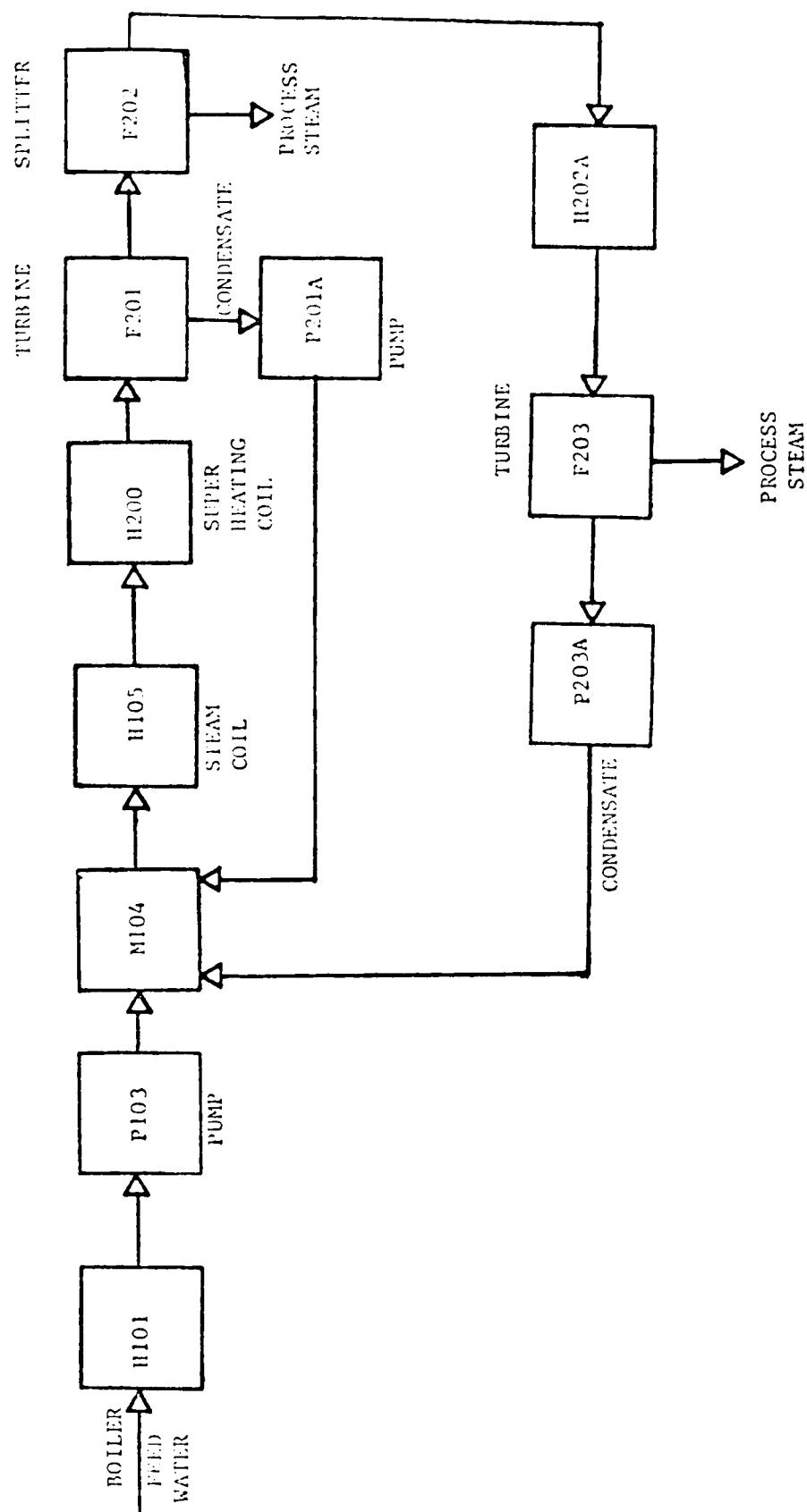


Figure 4.8. ASPEN flow-sheet for steam balance in conventional process

ASPEN program is run to determine the power requirements for the syn-gas compressors by inputting the necessary process data obtained from the earlier results. The total heat duty required to drive the syn-gas compressors is found to be 75.68 million BTU per hour.

The power requirement for the other miscellaneous drives is taken from the literature. It is reported that natural gas based ammonia plants require about 50 kwh of electric power per ton of ammonia (36). Considering a thermal efficiency of 35 percent, the total heat load for the power generation is estimated as 20.32 million BTU per hour for the present plant producing 41.667 tons of ammonia per hour.

The ASPEN results for different streams are given in Appendix A-IV. It is observed that the process steam streams S108 and S110 are carrying steam at the rates of 66,324 lb/hr and 29,365 lb/hr respectively and these are found to be in good agreement with the process requirements. ASPEN results for different heaters are presented in Figure 4.9. It can be observed that the heat loads for the feed water heater, steam coil and superheating coils (H200 and H202A) are 13.39, 160.10 and 40.56 million BTU per hour, respectively.

The ASPEN results obtained so far will enable us to arrive at the total heat load of the furnace. The heat loads for the different units are summarized in Table 4.4. It can be observed that the total fuel requirement for the furnace is 472 million BTU per hour. It is found earlier that the natural gas feed requirement

GENERAL-HEAT (HEATER): H101

INPUT STREAM: S101

OUTPUT STREAM: S102

PROPERTY OPTION SET SYSOP5

*** RESULTS ***

OUTPUT TEMPERATURE	F	190.00
OUTPUT PRESSURE	PSI	50.000
HEAT DUTY	BTU/HR	.13385D+08
VAPOR FRACTION		.0

GENERAL-HEAT (HEATER): H105

INPUT STREAM: S104A

OUTPUT STREAM: S105

PROPERTY OPTION SET SYSOP5

*** RESULTS ***

OUTPUT TEMPERATURE	F	600.00
OUTPUT PRESSURE	PSI	1500.0
HEAT DUTY	BTU/HR	.16010D+09
VAPOR FRACTION		1.0000

GENERAL-HEAT (HEATER): H200

INPUT STREAM: S105

OUTPUT STREAM: S105A

PROPERTY OPTION SET SYSOP12

*** RESULTS ***

OUTPUT TEMPERATURE	F	900.00
OUTPUT PRESSURE	PSI	1500.0
HEAT DUTY	BTU/HR	.32589D+08
VAPOR FRACTION		1.0000

GENERAL-HEAT (HEATER): H202A

INPUT STREAM: S109

OUTPUT STREAM: S109A

PROPERTY OPTION SET SYSOP12

*** RESULTS ***

OUTPUT TEMPERATURE	F	750.00
OUTPUT PRESSURE	PSI	566.15
HEAT DUTY	BTU/HR	.79654D+07
VAPOR FRACTION		1.0000

Figure 4.9. Heat loads for steam generation--Conventional process

TABLE 4.4
REFORMER FURNACE HEAT LOAD

Item	Heat load MM Btu/hr
Feed pre-heater	11.54
Air pre-heater	14.13
Endothermic reaction	232.00
Boiler feed water pre-heater	13.39
Steam coil	160.10
Super heating coils	40.56
Total heat load	471.72

for this plant is 740,645 scf/hr. Considering a heating value of 1020 btu/scf for the natural gas, the feed gas requirement will be 755.46 million BTU per hour. From the above, it can be seen that the total requirement of natural gas (feed+fuel) for this plant is 1227.46 million BTU per hour. Further, if we consider a 5 percent total losses due to wastes and leaks, the total gas requirement can be estimated as 1289 million BTU per hour. It is reported that a plant producing 1000 tons of ammonia per day will have a gas requirement of 1291 million BTU per hour (8). From this it can be concluded that the data obtained in the present study is in good agreement with the above.

4.2 Coal--Ammonia

As mentioned earlier, coal has been considered as a potential alternative feedstock for producing ammonia. This non-conventional process is also simulated using ASPEN.

4.2.1 Material balances

The important manufacturing stages shown earlier in Figure 3.2 are modeled with various unit operation blocks available in ASPEN. The process flow scheme simulated by ASPEN is given in Figure 4.10. Coal is a non-conventional compound and is not included in the property data in the data sets of ASPEN data bank. A special kind of input data needs to be specified for all non-conventional materials. ASPEN contains different types of component attributes and enthalpy models through which the necessary data can be supplied. Some of these are Proxanal for the proximate analysis,

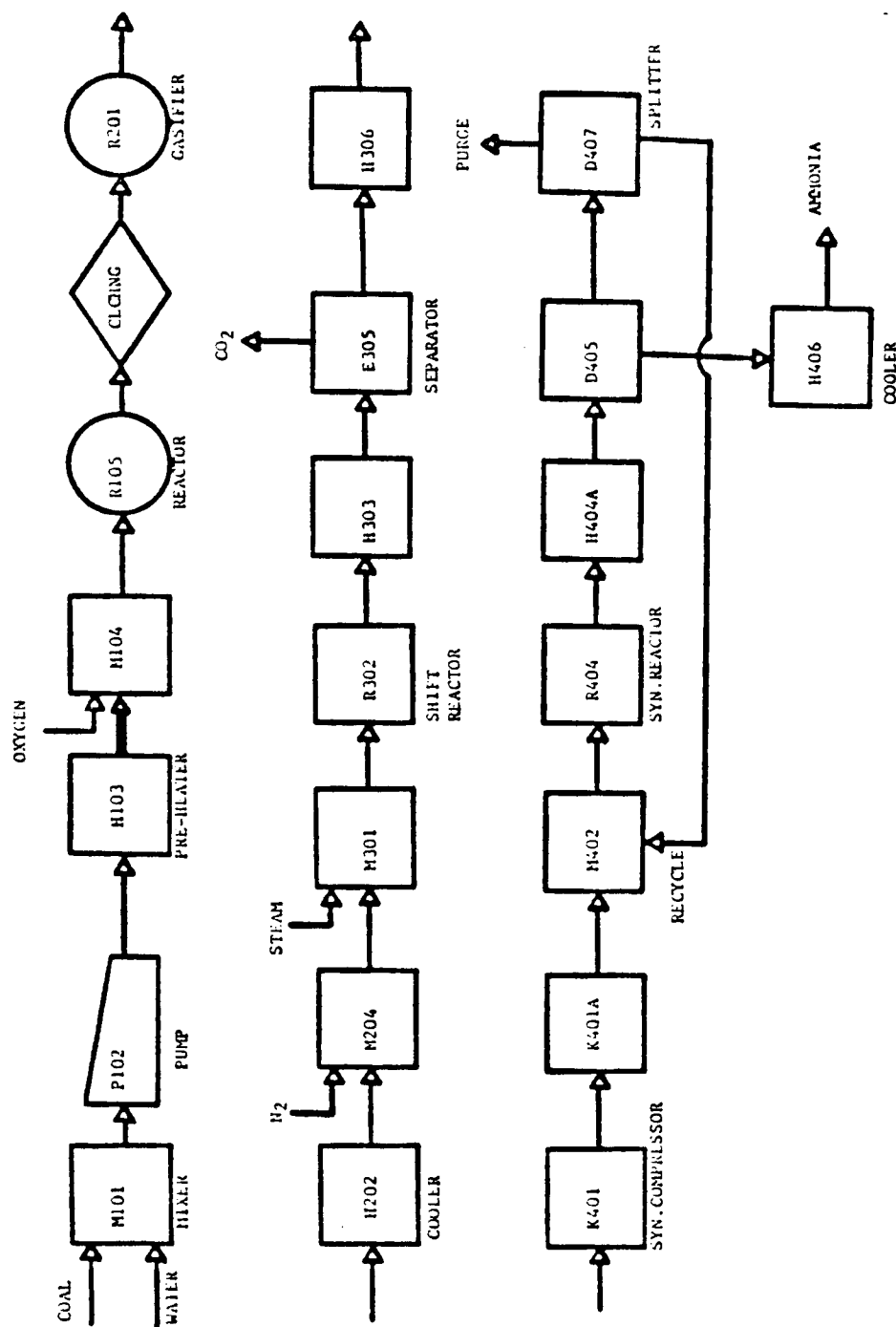


Figure 4.10. Flow scheme for ASPEN simulation--Non-conventional process for manufacturing ammonia from coal

Ultanal for the ultimate analysis, Sulfanal for the sulfur analysis, Aoxanal for the ash oxide analysis and Coalmisc for miscellaneous coal properties. In the present case, different constituents of coal are supplied through Ultanal and Proxanal. For the enthalpy of coal, the Boie heat of combustion correlation is used. As indicated earlier, Illinois No.6 coal is considered for the present study. The analyses are taken from the literature (37) and used as input. Table 4.5 gives the above analyses representing the various components in the order given for the data input. The method to input this data is given in the Appendix B-I along with the other ASPEN code for simulating the entire flow sheet.

In the present study, coal gasification is done through a Texaco gasifier. The feed for this gasifier will be in the form of slurry. In the ASPEN flow sheet (see Figure 4.10) coal and water are mixed in a mixer block M101 and pre-heated in a heater H103. Oxygen required for the gasification reactions is mixed with the above and sent to the gasifier. The gasifier is modeled as two reactors R105 and R201. It is assumed that in the first reactor all the carbon in the coal is converted into carbon monoxide, which further reacts with excess oxygen to form carbon dioxide. This first reactor is modeled as a stoichiometric reactor to simulate the supplied stoichiometry. So far, the flow sheet deals mainly with the non-conventional compounds and is in the non-conventional mode. This is to be converted into the conventional mode to carry out the simulation for the rest of the flow sheet, which contains mainly conventional compounds. This is achieved by connecting the

TABLE 4.5
ANALYSES FOR ILLINOIS NO.6 COAL

Element	Weight percent
Ultimate analysis	
Ash	9.7
Carbon	66.3
Hydrogen	4.8
Nitrogen	1.2
Chlorine	0.0
Sulfur	3.9
Oxygen	11.1
Proximate analysis	
Moisture	10.2
Fixed carbon	46.0
Volatile matter	34.7
Ash	9.1

Source: Elliott, M.A, Chemistry of Coal Utilization, John Wiley and Sons, New York, 1981, p. 1626.

two reactors with a block CLCHNG which changes the class of the flow sheet from non-conventional to conventional. To simulate chemical equilibrium at the exit conditions of the Texaco gasifier the second reactor is modeled as an equilibrium reactor wherein the carbon monoxide further reacts to form carbon dioxide and hydrogen. The process conditions selected can be seen from the ASPEN code in Appendix B-I. For the first reactor, the stoichiometry is worked out on 10 kg coal basis. ASPEN will calculate the production rates for various components as per that basis. The Texaco gasifier (R201) outlet stream composition for the major components is presented in Table 4.6 and compared with the literature (9). It is observed that the results obtained in this study are in good agreement.

The product gas from the gasifier is cooled and the nitrogen required for the synthesis is added. The steam for the shift reactor is mixed in a mixer M301. The water gas shift reaction is carried out in a stoichiometric reactor represented by R302. In the non-conventional process of producing ammonia, the acid gas and carbon dioxide removal is achieved by Rectisol process (6). The unit operation block E305 represents this separation. The syn-gas compression is represented by blocks K401 and K401A. The synthesis reactor is considered as a stoichiometric reactor R404. Part of the the recycle gas is purged through a splitter D407. The product ammonia vapors are cooled in H406 and sent to storage. The process conditions for the above are similar to the conventional process discussed earlier.

TABLE 4.6
OUTLET STREAM DATA FOR TEXACO GASIFIER

Component	Flow rate lb-mole/hr	Percent	
		present work	literature (9)
Hydrogen	3,424	24.38	23.80
Carbon monoxide	4,409	31.40	30.60
Carbon dioxide	1,768	12.59	12.90
Water	4,256	30.30	30.30
Nitrogen	48	0.34	0.36
Hydrogen sulfide	136	0.97	1.01

The main inputs and outputs for the present flow sheet are given in Table 4.7. The data obtained for various streams are presented in Appendix B-II. It is observed that the production rate of ammonia in this flow sheet (product stream S409) is 993 tons per day.

4.2.2 Steam and Energy balances

The steam and energy balances for the non-conventional process are performed along lines similar to the earlier conventional process. The balances are done using two different ASPEN simulations. First, the Texaco gasifier is simulated to assess the heat available from the various gasification reactions. The heat loads required for major drives are taken from the results of main flow sheet (Figure 4.10) simulation. A separate steam balance flow sheet is developed to produce the steam required for the shift reactor and for the major drives.

The Texaco gasifier is simulated as per the ASPEN flow sheet shown in Figure 4.11. Oxygen is preheated in a heater and supplied to the gasifier along with the coal slurry. The gasifier is modeled as a stoichiometric reactor. The ASPEN code showing the necessary stoichiometry is given in Figure 4.12. This stoichiometry is based on 10 lb of coal feed to the reactor. The effluent from the gasifier is cooled in the heater block H106. The composition of the main components in the outlet stream from the gasifier is found to be in good accordance with the data presented earlier in Table 4.6. The heat loads obtained from the ASPEN results are also given in Figure 4.12. The total heat available is found to be around 190 million Btu per hour.

TABLE 4.7

MAIN INPUT AND OUTPUT STREAMS--NON-CONVENTIONAL PROCESS

Input	Output	Stream	Flowrate
stream ID	stream ID		
S101		Feedstock (Coal)	56.478 tons/hr
S102		Water for coal	92,436 lb/hr
		slurry	
S106		Oxygen for	3,725 lb-mole/hr
		gasifier	
S207		Nitrogen for	2,480 lb-mole/hr
		synthesis	
S301		Steam for	38,906 lb/hr
		shift reactor	
	S409	Ammonia	993 tons/day
		product	

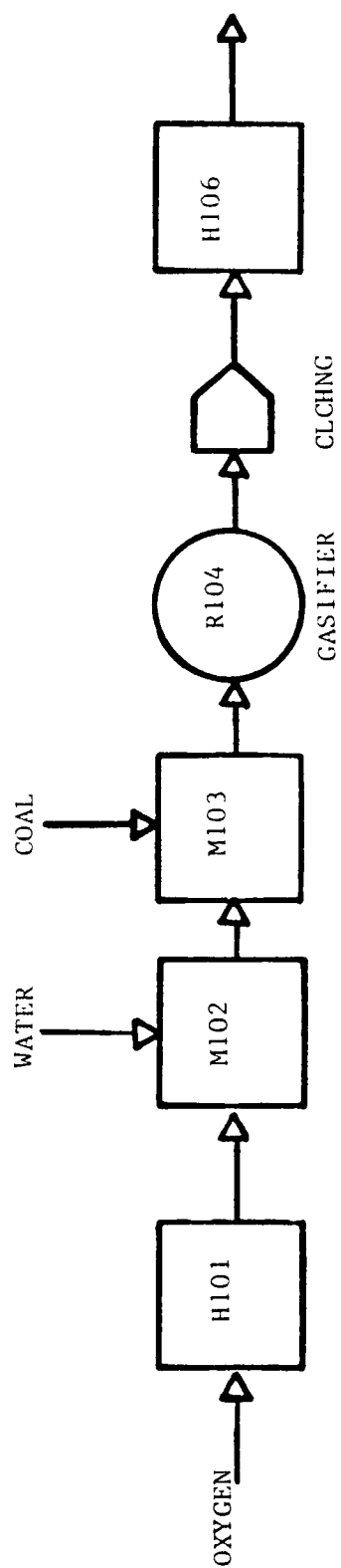


Figure 4.11. ASPEN flow diagram for Texaco gasifier simulation

```

BLOCK  R104  RSTOIC
PARAM  TEMP=1800  PRES=865.0
STOICH 1 NC COAL -10.0/MIXED O2 -.29121 /MIXED H2O -.0639 /
        MIXED CO .3883/MIXED CO2 .1637/MIXED H2 .302/
        MIXED N2 .00487
CONV 1 NC COAL 1.0

```

```

***  RESULTS  ***
REACT-STOICH (RSTOIC):  R104

OUTPUT TEMPERATURE  F 1800.0
OUTPUT PRESSURE     PSI 865.00
HEAT DUTY           BTU/HR -.16519D+09
VAPOR FRACTION                      .77884

GENERAL-HEAT (HEATER):  H106

OUTPUT TEMPERATURE  F 1600.0
OUTPUT PRESSURE     PSI 865.00
HEAT DUTY           BTU/HR -.26549D+08
VAPOR FRACTION                      .81024

```

Figure 4.12. ASPEN code and results for Texaco gasifier

The drives for various compressors are the major equipment using steam. The major compressors include the syn-gas compressors, oxygen compressor, nitrogen compressor and refrigeration compressor. Individual heat loads to drive these compressors are assessed from the ASPEN results and the total heat load is found to be 122.16 million BTU per hour. As indicated earlier, the steam requirement for the shift reactor is 2161.5 lb-mole/hr. A steam generation simulation is performed similar to the earlier flow sheet shown in Figure 4.8. Steam at 1500 psi and 900 degree F (superheated steam) is generated and passed through a turbine. Various compressors are driven by different turbines. However, the total load for all these turbines is approximated by treating as a single turbine system. A bleed stream is taken from this turbine for the process steam requirements (for shift reactor). The various heat loads required to produce the steam are found from ASPEN results. They are, 4.68 million Btu/hr for feed water heating, 121.84 million BTU/hr for the steam coil and 40.46 million Btu/hr for the superheating coil. The total heat load is approximately 167 million BTU/hr. It is reported that heat recovery in the Texaco gasifier is poor (38). Considering 85 percent heat recovery, the total heat load for the steam generation will be around 190 million BTU/hr. This figure is close to the amount of heat available from the Texaco gasifier. The power required for other miscellaneous purposes will be purchased from outside agencies. The cost involved in this will be discussed in a later chapter.

4.3 Atmospheric Fluidized Bed Combustor (AFBC)

One of the alternative arrangements considered to replace the conventional reformer furnace is the atmospheric fluidized bed combustor (AFBC). It is shown earlier that the heat load for the reformer furnace is 472 million BTU per hour (see Table 4.4). The coal feed rate to the AFBC and the lime stone (which is supplied along with coal to control sulfur dioxide emissions) consumption are calculated for the above heat load. The feed rates of coal and lime stone are found to be 30 tons/hr and 9.42 tons/hr respectively. The limestone rate is based upon a factor of 2.5 times the stoichiometric requirement for reaction with sulfur in the coal feed to the AFBC. The heat transfer area for the reformer catalyst tubes and the volume available for the catalyst are also checked and found to be adequate. These calculations are presented in Appendix C. An ASPEN simulation is performed for the AFBC to check the heat load for the above coal feed rate.

The ASPEN flow sheet for the AFBC simulation is shown in Figure 4.13. Air is formed by mixing nitrogen and oxygen in the correct proportions. The pre-heating of air to a temperature of 550 degree F is done in a heater block H102. Dried coal and hot air are mixed and sent to the combustor. The fluidized bed combustor is modeled with a stoichiometric reactor, R201. The ASPEN code showing the stoichiometry used to simulate the AFBC is given in Figure 4.14. The component attribute data input for the non-conventional

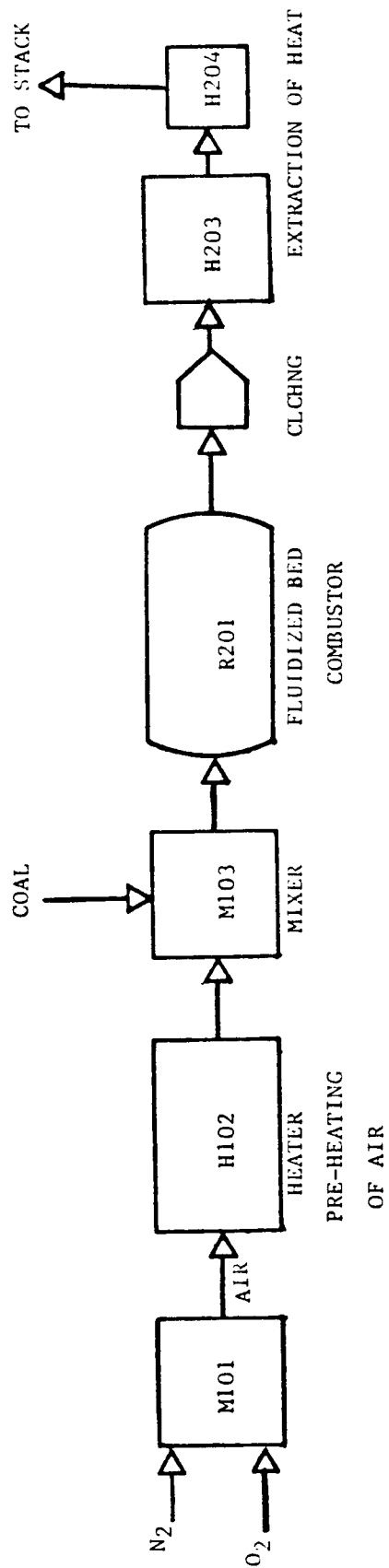


Figure 4.13. ASPEN flow sheet for Fluidized Bed Combustor

```

BLOCK  R201  RSTOIC
      PARAM  TEMP=1600  PRES=28.0
;IT IS ASSUMED THAT ALL CARBON IS BURNED TO FORM CARBONDIOXIDE, 90%S
;CAPTURE BY LIME.
      STOICH 1 NC COAL -10.0 / MIXED O2 -0.6780 /
      MIXED H2O  0.24 /      MIXED CO2 0.5525 / MIXED SO2 0.001219
;THE COMBUSTION PRODUCTS INDICATED ABOVE ARE ON A 10.0 LB COAL BASIS
      CONV 1 NC COAL 1.00

```

*** RESULTS ***

REACT-STOICH (RSTOIC): R201

OUTPUT TEMPERATURE	F	1600.0
OUTPUT PRESSURE	PSI	28.000
HEAT DUTY	BTU/HR	-.47197D+09
VAPOR FRACTION		1.0000

Figure 4.14. ASPEN code and results for AFBC simulation

material are similar to those used in the previous ASPEN code. The results obtained from the ASPEN for the heat load are also shown in Figure 4.14. It is observed that the heat load from the combustor for 30 ton per hour coal input is 472 million BTU per hour.

4.4 Medium Btu Gasifier

The second alternative fuel considered for the replacement of natural gas fuel in the primary reformer is Medium Btu Gas (MBG), generated from a Babcock and Wilcox gasifier. The coal input required to produce MBG for a heat duty of 472 million btu per hour is calculated from the data given in the literature (27). The coal consumption is estimated as 57,220 lb/hr. The quantity of steam and oxygen that are to be supplied to the gasifier are calculated as per the performance data reported for Babcock and Wilcox gasifier in the literature (37). The mass ratios of steam to coal and oxygen to coal considered in this study are 0.18 and 0.88 respectively.

The gasifier is simulated with the help of ASPEN to assess the amount of heat available during the process of generating MBG. The gasifier simulation is performed in a manner similar to the Texaco gasifier simulation (see Figure 4.11). The gasifier is modeled as a stoichiometric reactor and the raw gas is cooled in a heater block. The amount of heat available as process steam is found to be 73.4 million BTU per hour. The stoichiometry used to simulate the gasifier and the ASPEN results for the heat load are presented in Figure 4.15. The outlet stream composition of the gasifier and it's comparison with data presented in the literature (27) are given in Table 4.8. It is observed that the results obtained from the simulation are in reasonable agreement with the literature.

```

BLOCK R104 RSTOIC
  PARAM TEMP=1700 PRES=80.0
  STOICH 1 NC FOAL -10.0/MIXED O2 -.26/MIXED H2O -.0016/
        MIXED CO .4811/MIXED CO2 .0598/MIXEDH2 .2458/
        MIXED N2 .00487
  CONV 1 NC COAL 1.0
;THE GASIFICATION PRODUCTS INDICATED ABOVE ARE ON A 10 LB COAL BASIS
          *** RESULTS ***
REACT-STOICH (RSTOIC): R104
  INPUT STREAM: S106
  OUTPUT STREAM: S107
  PROPERTY OPTION SET SYSOP1

  OUTPUT TEMPERATURE      F              1700.0
  OUTPUT PRESSURE         PSI             80.000
  HEAT DUTY               BTU/HR          -.68991D+08
  VAPOR FRACTION                      1.0000

GENERAL-HEAT (HEATER): H106
  INPUT STREAM: S108
  OUTPUT STREAM: S109
  PROPERTY OPTION SET SYSOP1

  OUTPUT TEMPERATURE      F              1600.0
  OUTPUT PRESSURE         PSI             80.000
  HEAT DUTY               BTU/HR          -.43951D+07
  VAPOR FRACTION                      1.0000

```

Figure 4.15. ASPEN code and results for Babcock and Wilcox gasifier

TABLE 4.8

OUTLET STREAM DATA FOR BABCOCK AND WILCOX GASIFIER

Component	Flow rate lb-mole/hr	Percent	Composition
		present work	literature(27)
Hydrogen	1,407	31.06	28.00
Carbon monoxide	2,753	60.77	65.00
Carbon dioxide	342	7.55	4.00
Nitrogen	28	0.62	1.00

The heat available from the gasifier is used to generate the steam. This steam is considered as a credit for the alternative system. An ASPEN simulation is used to find the quantity of steam that can be generated from the available heat. This simulation is performed similar to the previous steam generation simulations. Steam at 1500 psi and 900 degree F (superheated steam) is generated. These conditions are chosen similar to the previous steam generation conditions so that this steam can be used to supplement the turbine steam whenever necessary. The amount of steam available is found to be 53,065 lb/hr with conditions stated above.

CHAPTER V

CAPITAL AND OPERATING COSTS ESTIMATION

One of the objectives of the present study is to assess the cost of ammonia in future years with the alternative arrangements proposed earlier. The cost of ammonia with these arrangements is evaluated and compared. To find the cost of ammonia, the capital and operating costs are to be estimated for different processes. In this chapter, the capital and operating costs for the four different cases are presented.

5.1 Case A--Conventional process with natural gas as feed and fuel

The cost routines available in ASPEN are used to estimate the cost of some equipment items. The important equipment for which ASPEN is utilized are the primary reformer, heat exchangers, secondary reformer and synthesis gas compressors. The process data obtained from the previous ASPEN simulations in Chapter IV are supplied as the input data to estimate the cost of the equipment. ASPEN supplies the cost data for the base year 1979. In the present study all the cost estimates are prepared in 1983 dollars. The 1979 cost data from ASPEN are projected to 1983 dollars by using Chemical Engineering annual plant indices. The annual indices considered for various years are shown in Table 5.1.

The ASPEN input data for evaluating the cost of the natural gas feed pre-heater, primary reformer and syn-gas compressor are given in Figure 5.1. The heat duty data are as per the previous

TABLE 5.1
ANNUAL PLANT INDICES

Year	Index
1972	137.2
1973	144.1
1974	165.4
1975	182.4
1976	192.1
1977	204.1
1978	218.8
1979	238.7
1980	261.2
1981	297.0
1982	314.0
1983	318.6

Source: Chemical Engineering,
McGraw Hill, New York.

```

; COST OF HEAT-EXCHANGER FOR FEED PRE-HEATING
CBLOCK   HX1   COST-HEATEX
        PARAM  NSB=1  TYPE=2  SPRS=73.5  TPRS=470.5  TMAT=1
        SIZE-INPUT  HDY=11531857  TI1=1472  TO1=932  TI2=302  TO2=752
;
; COST OF PRIMARY REFORMER
CBLOCK   FURNACE  COST-FURNACE
        PARAM  TYPE=3  MAT=3
        SIZE-INPUT  QTOT=472D06  PRES=470
;COST OF SYN GAS COMPRESSOR
CBLOCK   SYNCOMP1  COST-COMPRESS
        PARAM  NSB=0  CTYP=2  NCMP=1
        SIZE-INPUT  TVF=208781  PS=294  POUT=1470  GHP=12767

```

Figure 5.1. ASPEN input data for evaluating the cost of different equipment

ASPEN simulation results. Guthrie (43,44) presented extensive equipment cost evaluations. In this study, some of the equipment costs are taken from the above data and projected to 1983 dollars. The costs of various equipment evaluated using ASPEN and the above literature (43,44) are presented in Table 5.2.

The process sections such as the shift section and synthesis section involve ancillary equipment in addition to major equipment like reactors. Models reported in the literature to estimate the cost of different sections of a plant are used to obtain a reasonably accurate estimate for the process sections. International Research and Technology Corporation (46) developed various investment cost models for different sections of ammonia plants. In the present study, these models are used to assess the installed cost of various equipment in the shift section, purification section and synthesis sections. The process data required for substituting in these models are taken from the ASPEN simulation results. Table 5.3 presents the cost estimates for the above sections projected to 1983 dollars.

To find out the installed cost of various equipment listed earlier in Table 5.2, other costs like piping, building, service facilities etc. are to be added. Peters and Timmerhaus (45) present factors for these costs in detail. In the present study, these factors (as percentage of purchased cost) are selected from the above. Table 5.4 gives the details for various items considered in this study. With these factors, the total capital investment for a plant producing 1000 tons of ammonia per day is estimated as 138.548 million dollars(1983).

TABLE 5.2
COST OF MAIN EQUIPEMENT--CONVENTIONAL PROCESS

S.NO	Item	Basis for costing	Cost 1983 dollars
1	Heat exchanger for feed preheating	ASPEN	24,000
2	Primary reformer	ASPEN	5,723,000
3	Secondary reformer	ASPEN	1,669,000
4	Desufurizer vessels	ASPEN	63,000
5	Syngas compressors	ASPEN	6,827,000
6	Turbine drive for compressors	Literature(44)	1,256,000
7	Air compressor with drive--sec.reformer	Literature(43)	507,000
8	Air preheater	ASPEN	697,000
9	Steam boiler	Literature(43)	1,359,000
10	Turbogenerator	Literature(43)	1,400,000

TABLE 5.3

COST ESTIMATES FOR DIFFERENT SECTIONS--CONVENTIONAL PROCESS

Section	Basis for using the model in the literature(46)	Investment 1983 dollars
Shift section	Molar flow rate, pressure and concen- trations of CO and H ₂	1,565,000
CO ₂ and methane removal	Molar flow rate	2,240,000
Synthesis section	Production rate of ammonia	25,397,000

TABLE 5.4

VARIOUS FACTORS SELECTED FOR TOTAL INVESTMENT

S.NO	Item	Percent on purchased cost
1	Installation	40.0
2	Insulation	8.0
3	Piping	66.0
4	Electrical installation	12.5
5	Cost of buildings	45.0
6	Yard improvements	15.0
7	Service facilities	65.0
8	Land	6.0
9	Engineering and supervision	30.0
10	Instrumentation	13.0
		Percent on total installed cost
11	Construction (during erection etc.)	7.0
12	Contractor's fee	5.0
13	Contingencies	8.0
14	Startup expenses	9.0

The cost of natural gas as feed and fuel, is the main operating cost in the conventional process. From the previous ASPEN simulation results, it is found that the total requirement of natural gas for this process is 1303 million BTU per hour. As the price of ammonia in future years is to be worked out in this study, the price of natural gas in future years is to be evaluated first. For this, a price model is developed from the prices of natural gas reported in the literature (24) for the recent years. These prices are projected to 1983 dollars by using the U.S consumer overall price index. The various indices considered for the recent years are presented in Table 5.5. Recent natural gas prices from the literature (24) and the projected prices in 1983 dollars are given in Table 5.6. The model developed from the above data is

$$\text{Price} = 765.4954 + 0.4318 * (\text{year}) - 213.0 * \ln(\text{year}) \quad (5.1)$$

where the price is dollars per million BTU of natural gas in 1983 dollars. The price of natural gas in future years from the above model is compared with the literature predictions (23) and shown in Figure 5.2. The predicted natural gas prices are presented in Table 5.7. From the comparison, it can be seen that the above model gives reasonably good values for the natural gas price in future years.

The initial catalyst cost and the yearly cost for their replacement are taken as per the literature (42). The initial cost of catalysts is estimated as 905,000 dollars (1983) and their yearly replacement cost is 342,000 dollars (1983). The cooling

TABLE 5.5

U.S. CONSUMER PRICE INDICES

Year	Index
1970	116.3
1971	121.3
1972	125.3
1973	133.1
1974	147.7
1975	161.2
1976	170.5
1977	181.5
1978	195.3
1979	217.6
1980	247.0
1981	272.3
1982	288.6
1983	297.8

Source: U.S.Dept.of Labor, Bureau
of Labor Statistics.

TABLE 5.6

NATURAL GAS PRICE IN RECENT YEARS

Year	Price of Natural Gas (\$/MM BTU)	
	current dollars	1983 dollars
1973	0.44	0.99
1974	0.60	1.21
1975	0.94	1.74
1976	1.36	2.38
1977	1.74	2.86
1978	1.79	2.73
1979	1.94	2.66
1980	2.64	3.18
1981	3.25	3.55
1982	4.08	4.21
1983	4.32	4.32

Source: Monthly Gas Utility Statistical Report,
American Gas Association,
Arlington, Virginia.

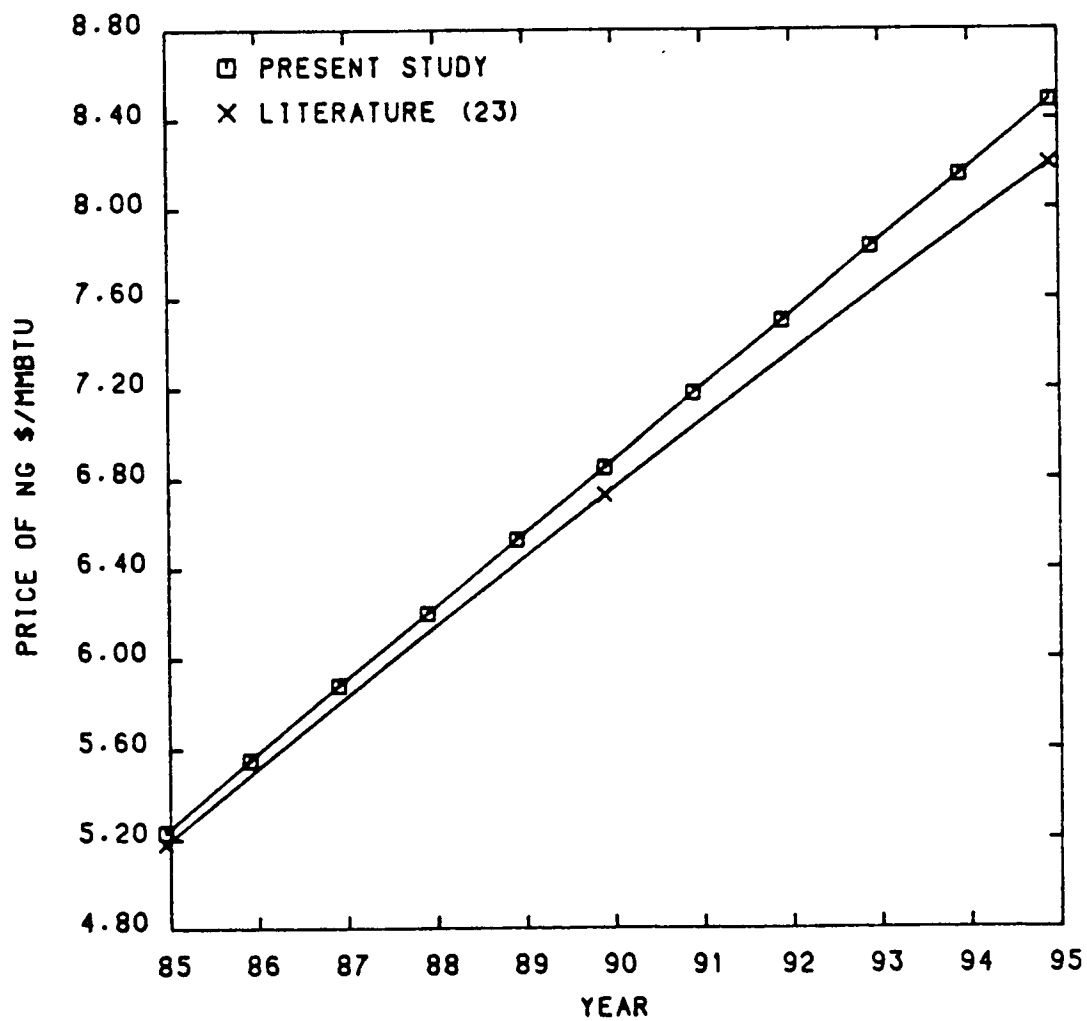


Figure 5.2. Price of natural gas (1983 dollars) in future years

TABLE 5.7
PREDICTED NATURAL GAS PRICE IN FUTURE YEARS
(1983 dollars)

Year	Price of Natural Gas (\$/MM BTU)	
	present work	literature(23)
1985	5.23	5.18
1986	5.55	
1987	5.88	
1988	6.20	
1989	6.53	6.73
1990	6.85	
1991	7.18	
1992	7.50	
1993	7.83	8.20
1994	8.15	
1995	8.48	

water and boiler feed water requirements are taken as per the literature (6). The cost involved in the water consumption is estimated as 2.11 million dollars (1983) per year on 330 working days basis. The plant will be self sufficient in steam and power generation. The maintenance and labor costs for the plant are taken as 3 percent (1.5 percent each) of the total capital investment.

5.2 Case B--Non-conventional process with coal as feed

The capital estimate for the non-conventional process using coal alone as feedstock gasified in a Texaco gasifier is made along lines similar to the previous estimate. A portion of the equipments' cost is estimated using ASPEN. Cost models reported in the literature (46) are used to evaluate the cost of some of the sections as in the previous estimate.

ASPEN is used to estimate the cost of the coal slurry pump, pre-heater, syngas compressors, oxygen and nitrogen compressors. The process data from the ASPEN simulations in the previous chapter are used to supply the necessary input data. The 1979 cost data obtained from ASPEN is projected to 1983 dollars using Chemical Engineering plant indexes as per the earlier Table 5.1. The cost of the drives for all the compressors is estimated as per the data by Guthrie(44). The costs obtained from ASPEN for various equipment are presented in Table 5.8 along with the cost for the drives from the literature (44).

TABLE 5.8

COST OF MAIN EQUIPEMENT--NON-CONVENTIONAL PROCESS

S.NO	Item	Basis for costing	Cost 1983 dollars
1	Slurry pump	ASPEN	73,000
2	Feed preheater	ASPEN	119,000
3	Syngas compressors	ASPEN	4,871,000
4	Turbine drive for compressors	Literature(44)	889,000
5	Oxygen compressor	ASPEN	2,437,000
6	Drive for the above compressor	Literature(44)	470,000
7	Nitrogen compressor	ASPEN	1,916,000
8	Drive for the above compressor	Literature(44)	364,000

The cost of coal preparation section is estimated as per the cost models and capacity exponents developed by International Research and Technology Corporation (46).. The entire coal preparation section is divided into five different sections and the cost estimation is made separately. The capital cost estimates for the synthesis section and air separation plant for producing oxygen and nitrogen are also as per the above models. For the cost estimation of the air separation plant, the volumetric flow rate and the outlet pressure of oxygen are to be supplied in addition to the capacity exponent. The capital cost involved in Texaco coal gasification units is estimated as per the cost estimates prepared by C.F.Braun and Company for Tennessee Valley Authority(TVA) (47). The cost involved in CO shift, acid gas removal and nitrogen wash using Rectisol process is estimated as per the literature (15). Various estimates for the above showing the capacity exponents considered in this study are presented in Table 5.9.

The installation factors for the equipments listed in Table 5.8 are considered as per the literature (45) and are listed in Table 5.4. These factors are applied to the purchased cost of the equipment and the installed cost of the total equipment is used to obtain the total capital investment. The total capital investment for the non- conventional process of producing 1000 tons of ammonia per day is estimated as 295.784 million dollars in 1983 dollars.

To assess the ammonia cost in future years, the cost of the raw material coal, is to be evaluated. To find the price of coal in future years, a price model is developed from the prices

TABLE 5.9

COST ESTIMATES FOR DIFFERENT SECTIONS--NON-CONVENTIONAL PROCESS

S.NO	Section	Capacity exponent/ basis	Investment 1983 dollars
1	Primary coal crushing	0.80	1,341,000
2	Coal stock- piling	0.62	6,970,000
3	Secondary coal crushing	0.80	917,000
4	Coarse coal feed preparation	0.80	1,940,000
5	Intermediate size coal feed preparation	0.60	4,840,000
6	Texaco gasifier	0.80	87,335,000
7	Oxygen plant	0.70	4,044,000
8	Shift and Rectisol processes	0.80	51,900,000
9	Synthesis	1000 TPD	25,397,000

reported in the literature (48,49) for the last 14 years. These prices are projected to 1983 dollars by using the price indexes given earlier in Table 5.5. The coal prices in recent years both in current dollars and 1983 dollars are given in Table 5.10. The cost model obtained from these data is

$$\text{PRICE} = -41629.54 + 32.54 * (\text{YEAR}) - 0.005774 * (\text{YEAR})^2 \quad (5.2)$$

where the price represents coal price in cents per million BTU, in 1983 dollars. The coal price in future years obtained from the above model is compared with the literature (22) and presented in Table 5.11. These two prices are also shown in Figure 5.3. From the comparison, it is observed that the above model gives reasonable predicted prices for coal in coming years. There is a discrepancy in the price during the initial period of time in Figure 5.3. However, it is expected from the recent coal price data that the coal prices will not increase sharply in near future.

The catalyst costs are taken as per the literature (15) and estimated as 573,000 dollars (1983) per year. The water requirement is 16 cubic meters per ton of ammonia (15) and at a cost of 34 cents per 1000 gallons, the water cost is estimated as 47,920 dollars (1983) per year on 330 working days basis. The electric power import from an outside agency is considered as 136 kwh per ton as per the literature (13). With the electric power cost at 5.90 cents per kwh (50), the total electric power cost is estimated as 2.71 million dollars (1983) per year on 330 working days basis. The maintenance and labor costs for the plant are taken as 3 percent of the total investment.

TABLE 5.10
COAL PRICE IN RECENT YEARS

Year	Price of Coal (c/MM BTU)	
	current dollars	1983 dollars
1970	20.40	52.24
1971	27.20	66.78
1972	29.90	71.06
1973	34.20	76.52
1974	40.00	80.65
1975	60.90	112.51
1976	85.60	149.51
1977	97.35	159.73
1978	100.79	153.69
1979	106.63	145.93
1980	125.64	151.48
1981	151.94	166.17
1982	164.15	169.38
1983	163.60	163.60

Source: 1). Coal Week, McGraw Hill, New York.
 2). Thomas, D.C, Economics of Synthetic Fuel Manufacture and Cost, TVA Report, Jan. 1980, p. 140.

TABLE 5.11
PREDICTED COAL PRICE IN FUTURE YEARS
(1983 dollars)

Year	Price of coal (\$/ton)	
	present work	literature(22)
1985	52.38	59.08
1986	55.28	
1987	57.68	
1988	60.08	
1989	62.48	
1990	64.85	65.40
1991	67.25	
1992	69.63	
1993	72.03	
1994	74.40	
1995	76.78	75.35

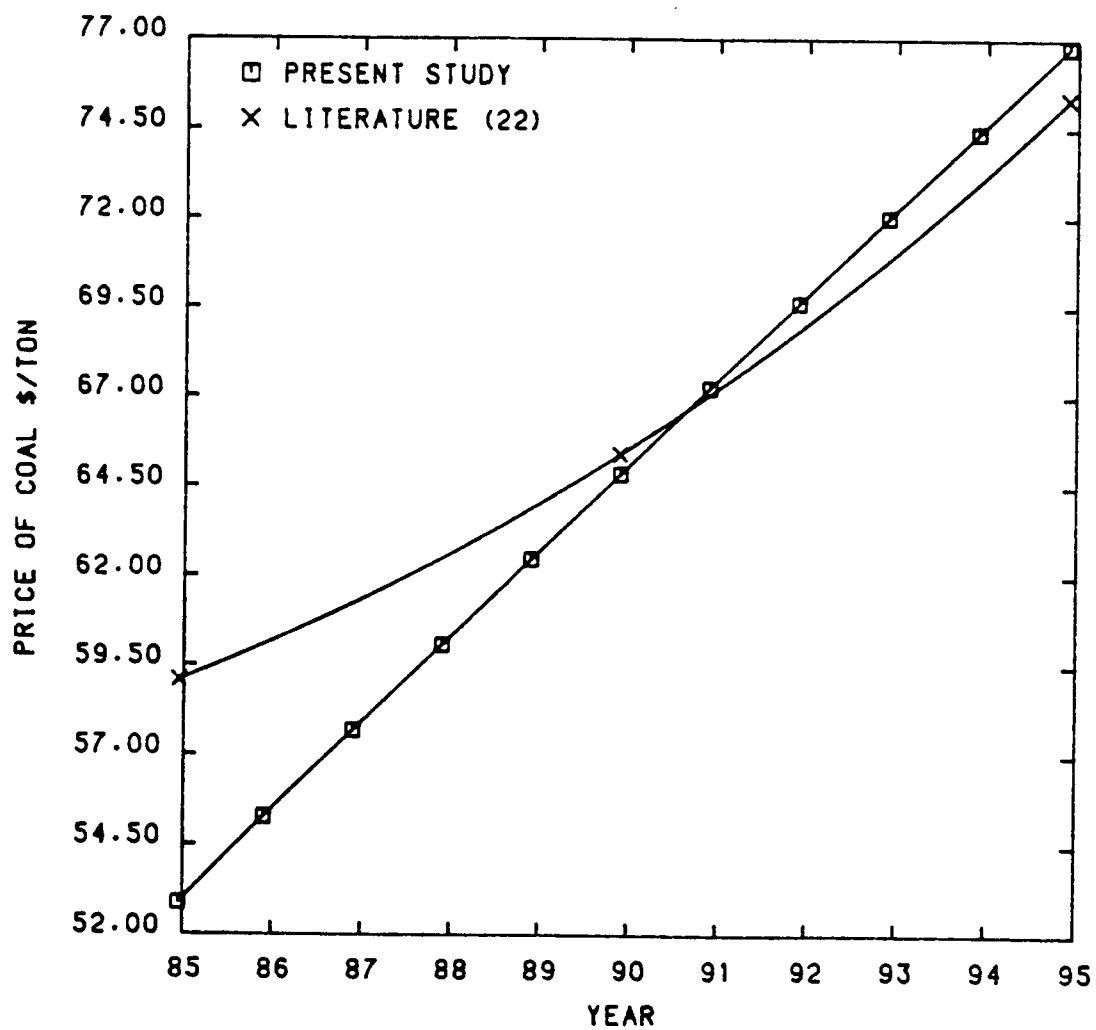


Figure 5.3. Price of coal (1983 dollars) in future years

5.3 Case C--Alternative arrangement with AFBC reformer

As indicated earlier, a coal-fired Atmospheric Fluidized Bed Combustor (AFBC) is considered as an alternative arrangement for the conventional reformer furnace. The cost estimates for this alternative arrangement have been made and the incremental capital and operating costs are developed.

The cost estimate for the AFBC plant is made by developing two different cost models, one for the combustor section and the other for the entire plant. Cost data for the AFBC reported in the literature (51-56) were collected and utilized to develop the models relating the required heat load and the capital cost. However, all of these cost data were for the power plants using AFBC boiler arrangements. Therefore to establish the cost of a process-oriented coal-fired AFBC reformer, the cost for boiler sections were separated and considered for the present study. As there is not much information reported in the literature regarding the cost of fluidized bed process heaters, the above method is used to find the cost. It can be established that the main components for both the arrangements (AFBC boiler and process heater) would be comparable and a reasonably accurate cost estimate for the process heater can be made from the cost data of boiler arrangements. Table 5.12 presents the data utilized for developing these models. The resulting models are:

Combustor plant:

$$\ln(Y) = -71.47166 + 25.26 \cdot \ln(X) - 2.826 \cdot (\ln(X))^2 + 0.1069 \cdot (\ln(X))^3 \quad (5.3)$$

TABLE 5.12

DATA FOR DEVELOPING COST MODELS FOR AFBC PLANT

Plant capacity MM BTU/HR	Capital Cost in million dollars (1983)		Literature source
	Combustor plant	Total plant	
288.8	1.52	5.72	(53)
1228.0	38.73	69.10	(51)
1344.0	47.53	303.18	(54)
3413.0	127.30	195.11	(55)
6192.0	97.95	155.27	(56)
9533.0	170.40	429.73	(52)

Total plant:

$$\ln(Y1) = -13.92082 + 3.749 * (\ln(X)) - 0.1721 * (\ln(X))^2 \quad (5.4)$$

where

X = Heat load in million BTU per hour

Y = Capital cost for combustor plant in million dollars (1983)

Y1 = Capital cost for total plant in million dollars (1983)

The above models have multiple regression coefficients of 0.9949 and 0.9924 respectively for the above equations 5.3 and 5.4.

For the present case, the AFBC total heat load is 472 million BTU per hour (see Table 4.4). The capital cost estimates for the AFBC plant are found to be 6.52 million dollars (1983) for the combustor and 13.98 million dollars (1983) for the total plant.

The coal and limestone consumption rates are as per the earlier calculations (see Appendix C). The price of coal in future years is taken as per the earlier model given by equation 5.2. The price of limestone is from the literature (57) and the limestone costs are estimated as 447,640 dollars (1983) per year (330 working days basis).

5.4 Case D--Alternative arrangement with MBG fuel for reformer

Medium BTU Gas (MBG) generated from a Babcock and Wilcox gasifier is considered as a second alternative fuel to replace the natural gas in the conventional primary reformer furnace. The cost estimates reported in the literature (27) for different Babcock and Wilcox gasifier capacities are utilized to evaluate the capacity exponent. The exponent is found to be 0.737. The capital cost

estimates for different sections are presented in Table 5.13. It is found that a plant producing 472 million BTU per hour of MBG requires a capital investment of about 68.633 million dollars (1983). The additional cost of renovations for the primary reformer to use the MBG as fuel is considered as 6 percent of this investment based upon a recent information (62).

The coal feed rate is taken from the ASPEN results. As indicated earlier, additional steam is generated in the gasifier while producing the MBG. This steam is considered as a credit for this type of arrangement. From the previous ASPEN results, it is found that 72,000 lb/hr of steam at 1500 psi and 900 degree F (superheated steam) is produced by the gasifier. From the enthalpy data of steam it is estimated that the above is equivalent to 78 million BTU/hr of heat energy. The amount of heat available is priced comparable to the natural gas price and considered as a credit for this alternative arrangement.

TABLE 5.13
COST ESTIMATE FOR MBG PLANT

Item	Cost in million \$ (1983)
Coal unloading, storage and handling	3.775
Coal preparation and gasification	17.158
Sulfur removal	5.491
Oxygen plant	20.933
Utilities and offsites	21.276
Total	68.633

CHAPTER VI

ECONOMIC ANALYSIS

One of the main objectives of the present study is to evaluate the cost of ammonia in future years with the various alternatives considered earlier. The process data obtained from the ASPEN simulations and the cost data from various cost routines and cost models were utilized to predict the cost of ammonia in coming years. The economics of substituting other fuels and feedstock for the natural gas in the conventional process for producing ammonia is studied with the help of Discounted Cash Flow (DCF). Various parameters considered in the base economic analysis to arrive at the cost of ammonia are presented in this chapter. A sensitivity analysis is made in this study by changing different parameters for various cases of interest. The details of this analysis and the predicted break even points in time for switching over to alternative fuel and feed arrangements are also presented in this chapter.

6.1 Base Economic Analysis

As indicated earlier, the discounted cash flow for various processes in the present study is performed with the help of CASHFLOW computer program. This program is run by supplying the necessary data in card format. The economic analysis is performed for the four processes to arrive at the cost of ammonia in each

case. The four different cases are:

Case A: Natural gas-Ammonia, a conventional process with natural gas as feed and fuel

Case B: Coal-Ammonia, a non-conventional process with coal as the feed gasified in a Texaco gasifier

Case C: Natural gas-AFBC-Ammonia, with natural gas as feed and a coal-fired AFBC reformer

Case D: Natural gas-MBG-Ammonia, with natural gas as feed and MBG as the fuel for reformer

The various parameters considered for the DCF analyses to produce 1000 tons of ammonia per day with the above processes are presented below.

6.1.1 Investment

The total investment for the different processes are taken from the cost estimates evaluated in Chapter V. The additional (incremental) costs involved in the Cases C and D are calculated and the total investments for these processes are found by adjusting the investment for the conventional process (Case A). The total investments are found to be 138.548, 295.784, 136.568 and 207.661 million dollars (1983 dollars) respectively for the Cases A, B, C and D.

6.1.2 Financial Criteria

The project life in all the cases is considered as 24 years with a 3 year construction period. The plants will operate with an efficiency of 60 percent, 70 percent and 80 percent respectively during the first, second and third years of operation and 90

percent thereafter. All the plants are considered to operate on a 330 working days per year basis. The Federal income tax is considered as 46 percent and the investment tax credit is taken at 7 percent. The tax losses are allowed to carry forward for a period of 5 years, however no negative Federal taxes are considered. A state income tax of 2 percent is also included. The interest rate on debt is considered as 9 percent. There will be no salvage value for the equipment after the project life.

The working capital includes 15 days of raw material, 15 days of labor, 10 days of product storage and 7 days receivables. The maintenance costs are taken as 3 percent with 50 percent each to materials and labor. The insurance charges are taken as 1 percent of the total investment for all the processes.

The base economic analysis is made by performing the discounted cash flow with Sum of the Years Digits (SYD) depreciation with a depreciable life of 16 years. The rate of return (ROR) on equity is considered as 10 percent after taxes. The debt to equity ratio is taken as 50 percent.

6.1.3 Raw materials

The raw material consumption rates are taken as per the results obtained earlier from the ASPEN simulations. In the CASHFLOW computer program all the input data are to be supplied for 100 percent on-stream efficiency. The product cost is calculated as per the efficiencies indicated for each year of operation. The natural gas consumption rate for the conventional process (Case A)

is found to be 11.414 million MMBTU per year with 100 percent stream efficiency. For the non-conventional process (Case B) the coal requirement is calculated as 0.449 million tons per year with 100 percent stream efficiency. In the first alternative arrangement (Case C) in which the conventional reformer is replaced with AFBC, the raw material requirements are found to be 7.2796 million MMBTU of natural gas per year and 0.2628 million tons of coal per year for 100 percent stream efficiency. For the alternative fuel MBG arrangement (Case D) the consumption of feedstocks are 7.2796 million MMBTU of natural gas per year and 0.2505 million tons of coal per year for full stream efficiency. The feedstock prices in future years are taken from the price models developed in the previous chapter. The MBG fuel arrangement (Case D) will have steam as an additional product. This is considered as a byproduct from the facility with a production rate of 0.6833 million MMBTU of heat energy per year (with 100 percent efficiency). This byproduct is assumed to provide a credit to this system and its' cost is equivalent to the natural gas price for the same amount of energy.

6.1.4 Results of Base Economic Analysis

With natural gas priced at \$ 5.23/MMBTU, the cost of ammonia is found to be 279.35 dollars per ton for Case A. The cost of ammonia for Case B is found to be 301.01 dollars per ton for a coal price of \$ 52.88 per ton. Case C and Case D predicted the cost of ammonia at \$ 257.63 and \$ 298.26 per ton respectively, with the same feedstock prices. The predicted prices of natural gas and coal

in future years obtained from the earlier models are used to find the cost of ammonia in future years in all the four cases. The cost of ammonia with different arrangements obtained from the discounted cash flow (DCF) analysis are presented in Table 6.1.

From these data, the alternative arrangement AFBC (Case C) is found to be the most interesting, with its low ammonia cost compared to the conventional process (Case A). The non-conventional process (Case B) also looks promising in coming years. The MBG fuel (Case D) doesn't offer immediate savings and appears to be economical only in the long run. To evaluate the effects of various other parameters on the cost of ammonia in different cases, a further study has been made using sensitivity analysis.

6.2 Sensitivity analysis

Sensitivity analysis is performed in this study to determine the effects of rate of return, type of depreciation and debt fraction on the price of ammonia in the different cases discussed above. As indicated earlier, the base analysis is made with SYD depreciation with 50 percent debt on investment and 10 percent rate of return on equity. The second type of depreciation considered is the Federal Accelerated Cost Recovery System (ACRS) (60). In this type of depreciation, the depreciable life is considered as 10 years. The total depreciable amount will be distributed over this 10 year period. The yearly charges are, 8 percent at the end of first year, 14 percent in the second year, 12 percent in the third year, 10 percent each on the next 3 years and 9 percent each on the

TABLE 6.1

COST OF AMMONIA IN FUTURE YEARS--BASE DCF WITH
10 PERCENT ROR AND 50 PERCENT DEBT TO EQUITY RATIO

(All in 1983 dollars)

Year	Price of NG	Price of Coal	Cost of ammonia \$/ton			
	\$/MM Btu	\$/ton	Case A	Case B	Case C	Case D
1985	5.23	52.88	279.35	301.01	257.63	298.26
1986	5.55	55.28	289.57	304.01	265.91	305.86
1987	5.88	57.68	300.10	307.03	274.39	313.64
1988	6.20	60.08	310.32	310.04	282.67	321.24
1989	6.53	62.48	320.86	313.06	291.15	329.02
1990	6.85	64.85	331.07	316.04	299.42	336.60
1991	7.18	67.25	341.61	319.05	307.90	344.39
1992	7.50	69.63	351.83	322.04	316.16	351.97
1993	7.83	72.03	362.36	325.05	324.65	359.75
1994	8.15	74.40	372.58	328.03	332.91	367.33
1995	8.48	76.78	383.12	331.02	341.37	375.10

remaining 4 years. The effect of debt financing is studied by increasing debt to equity ratio to 100 percent. For this total debt on investment it is considered that the debt repayment will be made through 12 equal yearly installment payments. The payments start from the fourth year when the plant goes on stream. The rate of return after taxes is always a matter of great interest to any investment. As such, the effect of increasing the rate of return after taxes to 15 percent is also studied. With all the above, eight different costs for ammonia are evaluated using the DCF for each of the four different cases. This means, that 32 different ammonia costs will result for each of the eleven future years 1985 to 1995. All these costs are arranged such that the effect of each variable can be studied and compared.

The cost of ammonia in future years is evaluated for SYD depreciation with 10 percent and 15 percent rates of return along with 50 percent debt to equity ratio for the Cases A and B. Table 6.2 presents the various costs obtained from the DCF. The data are also shown in Figure 6.1. It is observed that the non-conventional process (Case B) for ammonia production should be economically feasible in near future, since the cost of ammonia in Case A will be higher compared to Case B. With 10 percent of rate of return, Case B is observed to be competitive with Case A in the year 1988, at a price of around \$ 305 per ton of ammonia. When the rate of return on equity is increased to 15 percent, the switch over is found to be economical only after the year 1992.

TABLE 6.2

COST COMPARISON--CONVENTIONAL AND NON-CONVENTIONAL PROCESSES--DCF
WITH SYD DEPRECIATION AND 50 PERCENT DEBT TO EQUITY RATIO

Year	Cost of ammonia \$/ton (1983 dollars)			
	10% ROR		15% ROR	
	Case A	Case B	Case A	Case B
1985	279.35	301.01	303.90	361.79
1986	289.57	304.01	319.19	364.82
1987	300.10	307.03	329.79	367.86
1988	310.32	310.04	340.08	370.89
1989	320.86	313.06	350.69	373.93
1990	331.07	316.04	360.97	376.93
1991	341.61	319.05	371.58	379.96
1992	351.83	322.04	381.87	382.96
1993	362.36	325.05	392.47	386.00
1994	372.58	328.03	402.76	389.00
1995	383.12	331.02	413.37	392.00

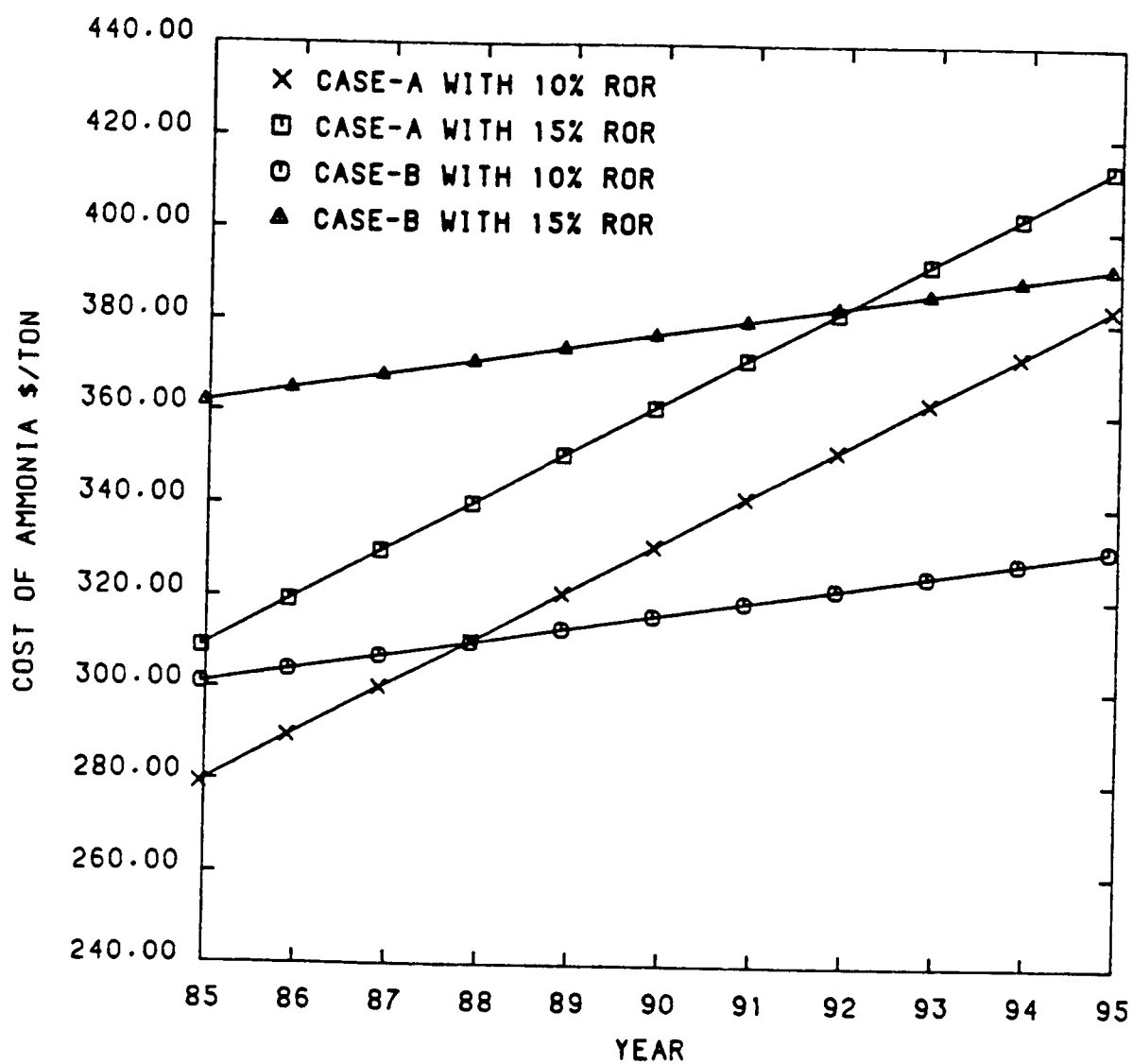


Figure 6.1. Ammonia cost comparison for Case A and Case B, DCF with SYD depreciation and 50 percent debt to equity ratio

Using the same type of depreciation (SYD) method, the debt to equity ratio is increased to 100 percent. The costs of ammonia for the two cases are shown in Table 6.3. Figure 6.2 also shows the trend of these costs. It can be seen that there is an increase in the cost of ammonia in both the cases over the previous costs with 50 percent debt to equity ratio. However the non-conventional process (Case B) will compete with the conventional process (Case A). The break even point in time is observed to occur in the years 1989 and 1992 respectively for 10 percent and 15 percent rates of return.

The analysis is performed using the ACRS depreciation in a manner similar to the above. The cost data obtained for 50 percent debt are presented in Table 6.4. The data are plotted in Figure 6.3. It is observed that there is a slight decrease in the price of ammonia when compared to the SYD depreciation. The break even is also found to occur slightly early when compared to the previous depreciation method. The ammonia costs with 100 percent debt to equity ratio and ACRS depreciation are presented in Table 6.5 and Figure 6.4. A cost increase of around 2.5 percent for Case A and 3.5 percent for Case B is observed. However, the non-conventional process (Case B) is found to be economical in coming years. The break even period is observed to be the same as before.

One of the interesting results observed in the present study is Case C, the alternative arrangement substituting the AFBC reformer for the primary reformer. The cost of ammonia with this arrangement is found to be less than the conventional process (Case A)

TABLE 6.3

COST COMPARISON--CONVENTIONAL AND NON-CONVENTIONAL PROCESSES--DCF
WITH SYD DEPRECIATION AND 100 PERCENT DEBT TO EQUITY RATIO

Year	Cost of ammonia \$/ton (1983 dollars)			
	10% ROR		15% ROR	
	Case A	Case B	Case A	Case B
1985	285.05	312.25	309.96	362.75
1986	295.30	315.27	320.29	365.79
1987	305.87	318.29	330.94	368.84
1988	316.11	321.32	341.27	371.88
1989	326.68	324.34	351.92	374.93
1990	336.92	327.33	362.25	377.94
1991	347.49	330.35	372.90	380.99
1992	357.73	333.34	383.23	384.01
1993	368.30	336.36	393.88	387.05
1994	378.55	339.36	404.21	390.07
1995	389.11	342.35	414.86	393.08

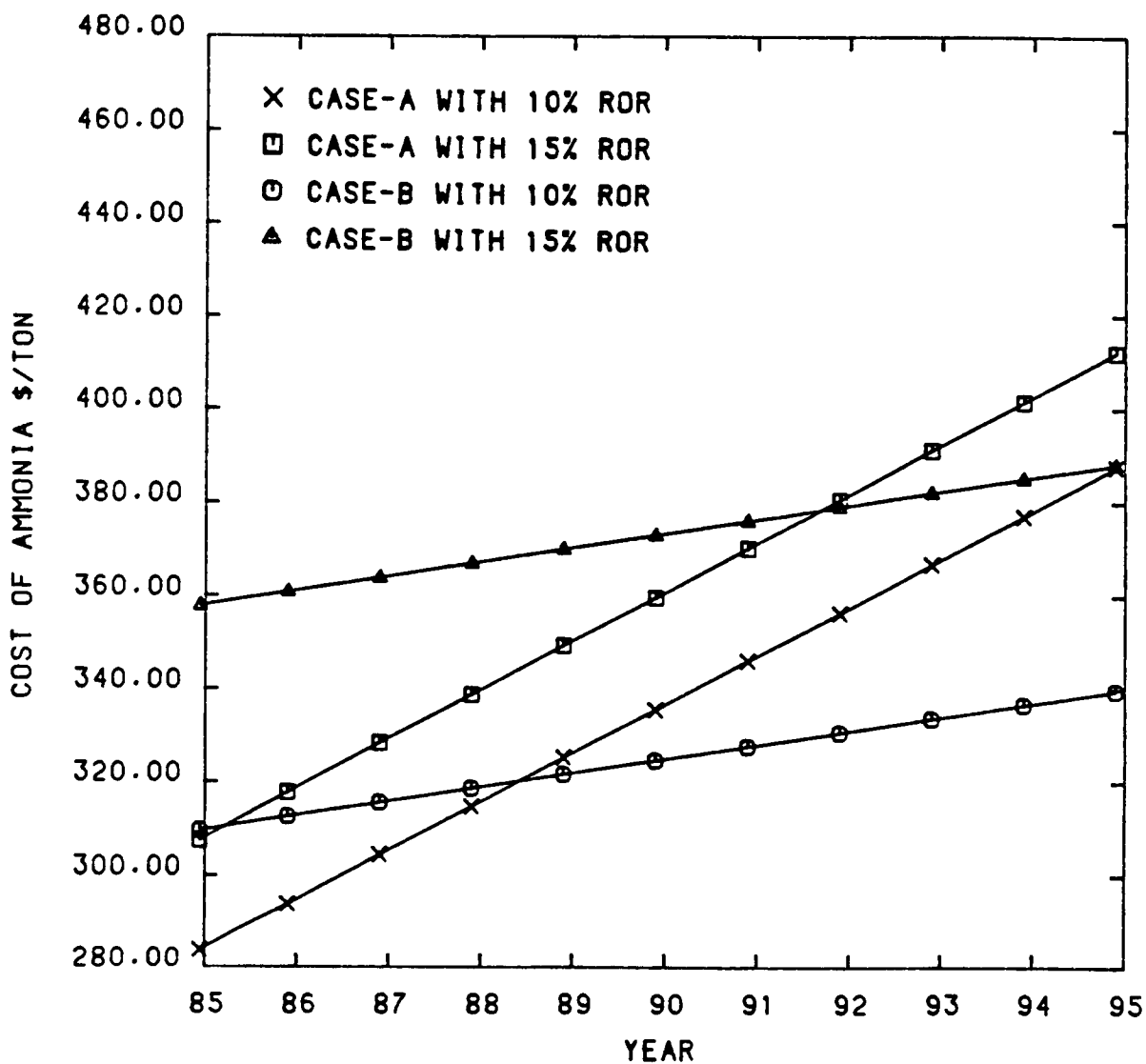


Figure 6.2. Ammonia cost comparison for Case A and Case B, DCF with SYD depreciation and 100 percent debt to equity ratio

TABLE 6.4

COST COMPARISON--CONVENTIONAL AND NON-CONVENTIONAL PROCESSES--DCF
WITH ACRS DEPRECIATION AND 50 PERCENT DEBT TO EQUITY RATIO

Year	Cost of ammonia \$/ton (1983 dollars)			
	10% ROR		15% ROR	
	Case A	Case B	Case A	Case B
1985	278.28	298.96	306.44	356.96
1986	288.49	301.97	316.71	359.98
1987	299.02	304.98	327.30	363.01
1988	309.23	307.99	337.58	366.04
1989	319.76	311.00	348.17	369.07
1990	329.97	313.98	358.44	372.07
1991	340.49	316.99	369.04	375.10
1992	350.70	319.97	379.31	378.10
1993	361.23	322.99	389.90	381.13
1994	371.44	325.97	400.19	384.13
1995	381.97	328.95	410.79	387.13

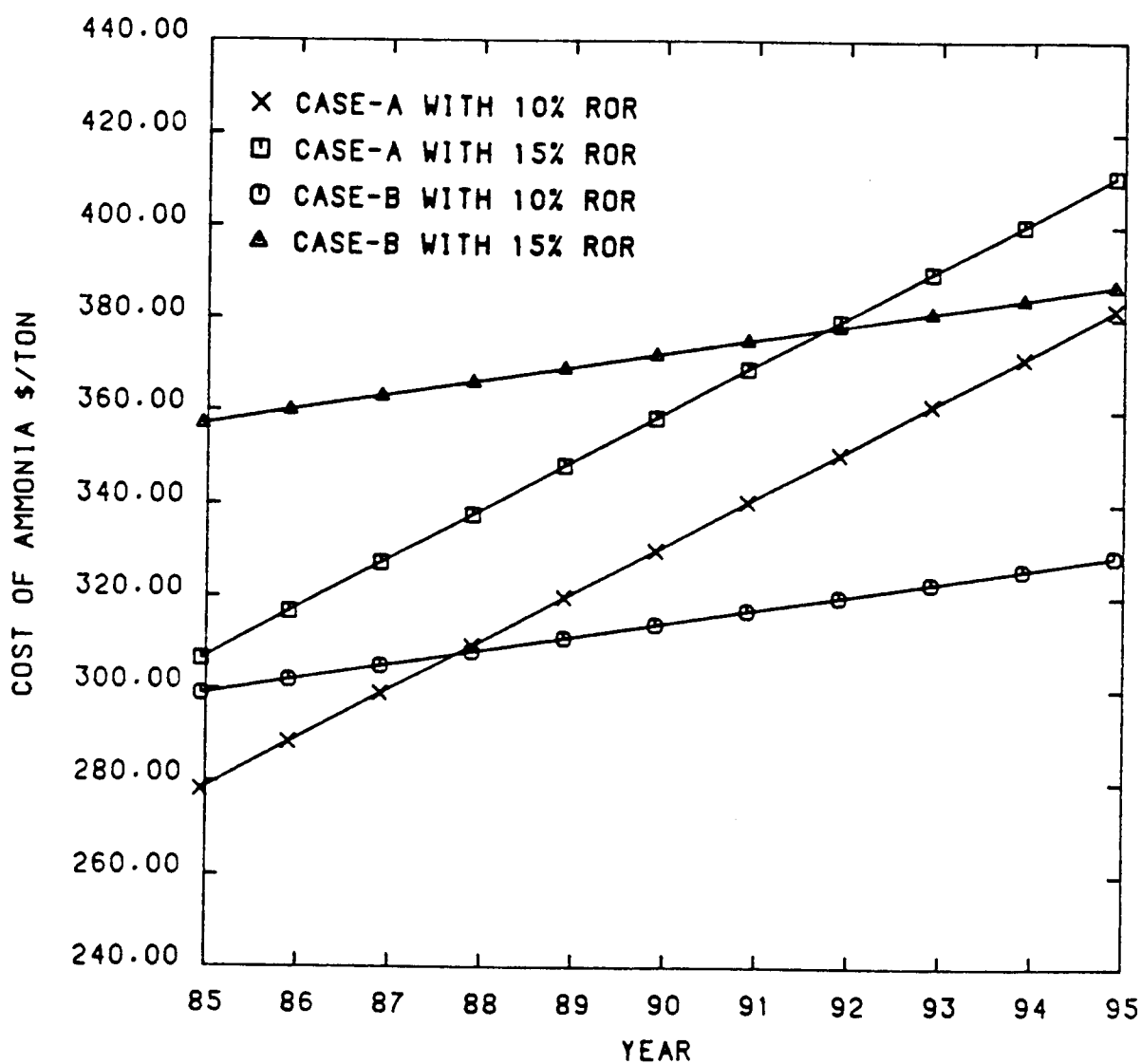


Figure 6.3. Ammonia cost comparison for Case A and Case B, DCF with ACRS depreciation and 50 percent debt to equity ratio

TABLE 6.5

COST COMPARISON--CONVENTIONAL AND NON-CONVENTIONAL PROCESSES--DCF
WITH ACRS DEPRECIATION AND 100 PERCENT DEBT TO EQUITY RATIO

Year	Cost of ammonia \$/ton (1983 dollars)			
	10% ROR		15% ROR	
	Case A	Case B	Case A	Case B
1985	283.65	309.56	307.39	357.80
1986	293.89	312.58	317.70	360.83
1987	304.44	315.60	328.33	363.87
1988	314.68	318.62	338.65	366.92
1989	325.24	321.64	349.28	369.96
1990	335.49	324.62	359.59	372.97
1991	346.05	327.64	370.23	376.01
1992	356.30	330.63	380.54	379.02
1993	366.87	333.65	391.17	382.06
1994	377.11	336.64	401.48	385.07
1995	387.68	339.63	412.12	388.08

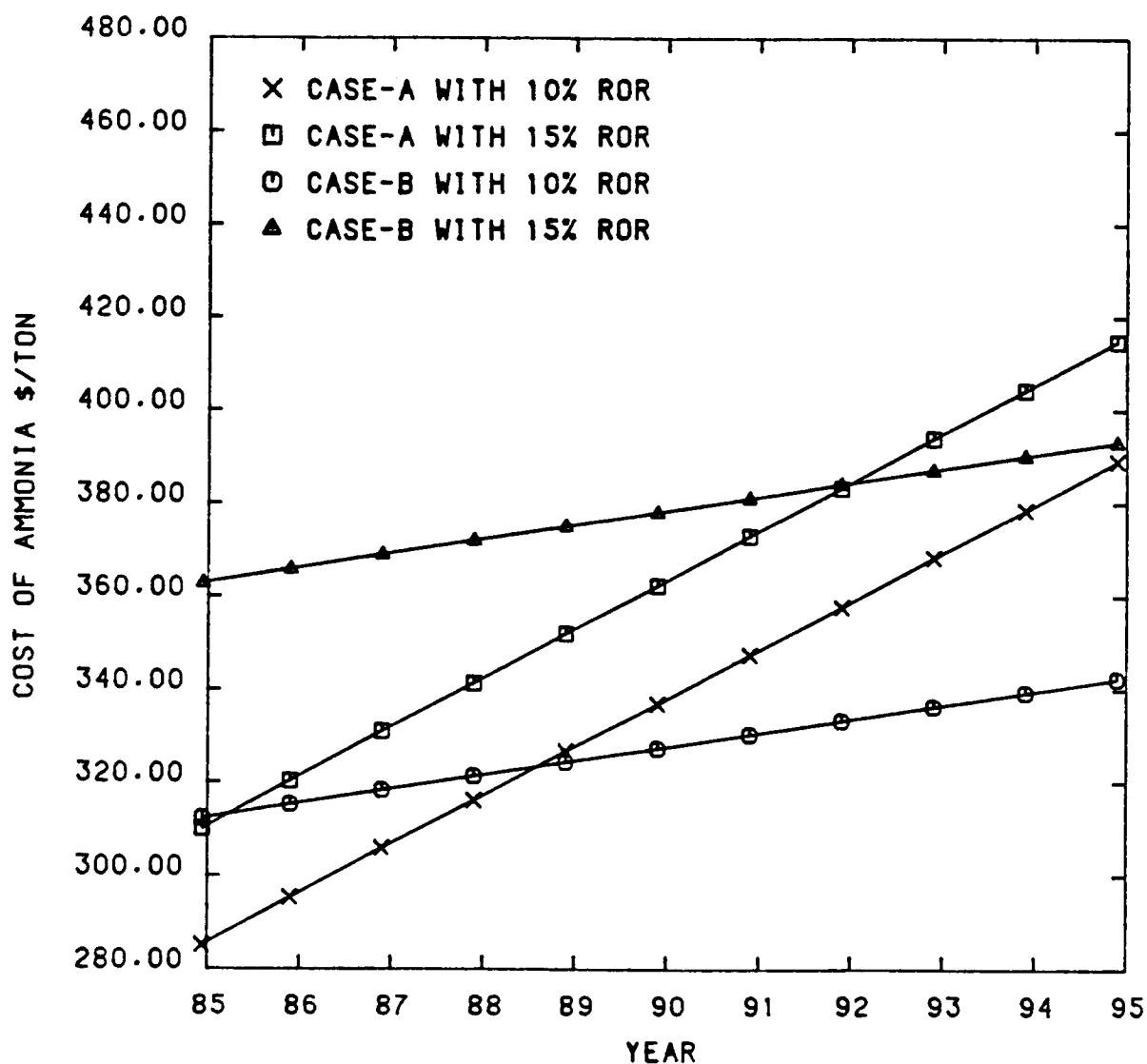


Figure 6.4. Ammonia cost comparison for Case A and Case B, DCF with ACRS depreciation and 100 percent debt to equity ratio

to an extent of about \$ 20 per ton. Table 6.6 presents the costs for this alternative arrangement with SYD depreciation and 50 percent debt to equity ratio. Figure 6.5 gives the comparison for the costs with 10 percent and 15 percent rates of return. It is observed that Case C is economical for both 10 percent ROR and 15 percent ROR, right from the year 1985. Table 6.7 and Figure 6.6 present the details for increased debt to equity ratio with the same depreciation method. The cost of ammonia has gone up by about 2 and 3 percent with 10 and 15 percent rates of return respectively. However, the costs are competitive with Case A.

The cost details with the second type of depreciation method (ACRS) are given in Table 6.8 and compared in Figure 6.7. The cost of ammonia with 50 percent debt on investment doesn't show any dramatic change compared to the cost by the previous depreciation method. It is observed that the costs are slightly less (about \$ 1.5/ton) compared to the previous one. Ammonia costs with 100 percent debt to equity ratio and ACRS depreciation are given in Table 6.9 and Figure 6.8. It is observed that the change in cost with 15 percent rate of return is very less, even though the debt ratio has been increased to 100 percent. As it can be observed from the plot, the cost of ammonia in Case C is less compared to Case A for all the years.

The second alternative fuel arrangement considered in the present study is Medium Btu Gas (MBG) as Case D. The cost of ammonia with this arrangement for the SYD depreciation and 50 percent debt to equity ratio are given in Table 6.10 and Figure 6.9.

TABLE 6.6

COST COMPARISON--CONVENTIONAL PROCESS AND AFBC ARRANGEMENT--DCF
WITH SYD DEPRECIATION AND 50 PERCENT DEBT TO EQUITY RATIO

Year	Cost of ammonia \$/ton (1983 dollars)			
	10% ROR		15% ROR	
	Case A	Case C	Case A	Case C
1985	279.35	257.63	308.90	286.64
1986	289.57	265.91	319.19	294.97
1987	300.10	274.39	329.79	303.51
1988	310.32	288.67	340.08	311.85
1989	320.86	291.15	350.69	320.39
1990	331.07	299.42	360.97	328.71
1991	341.61	307.90	371.58	337.25
1992	351.83	316.16	381.87	345.57
1993	362.36	324.65	392.47	354.11
1994	372.58	332.91	402.76	362.43
1995	383.12	341.37	413.37	370.95

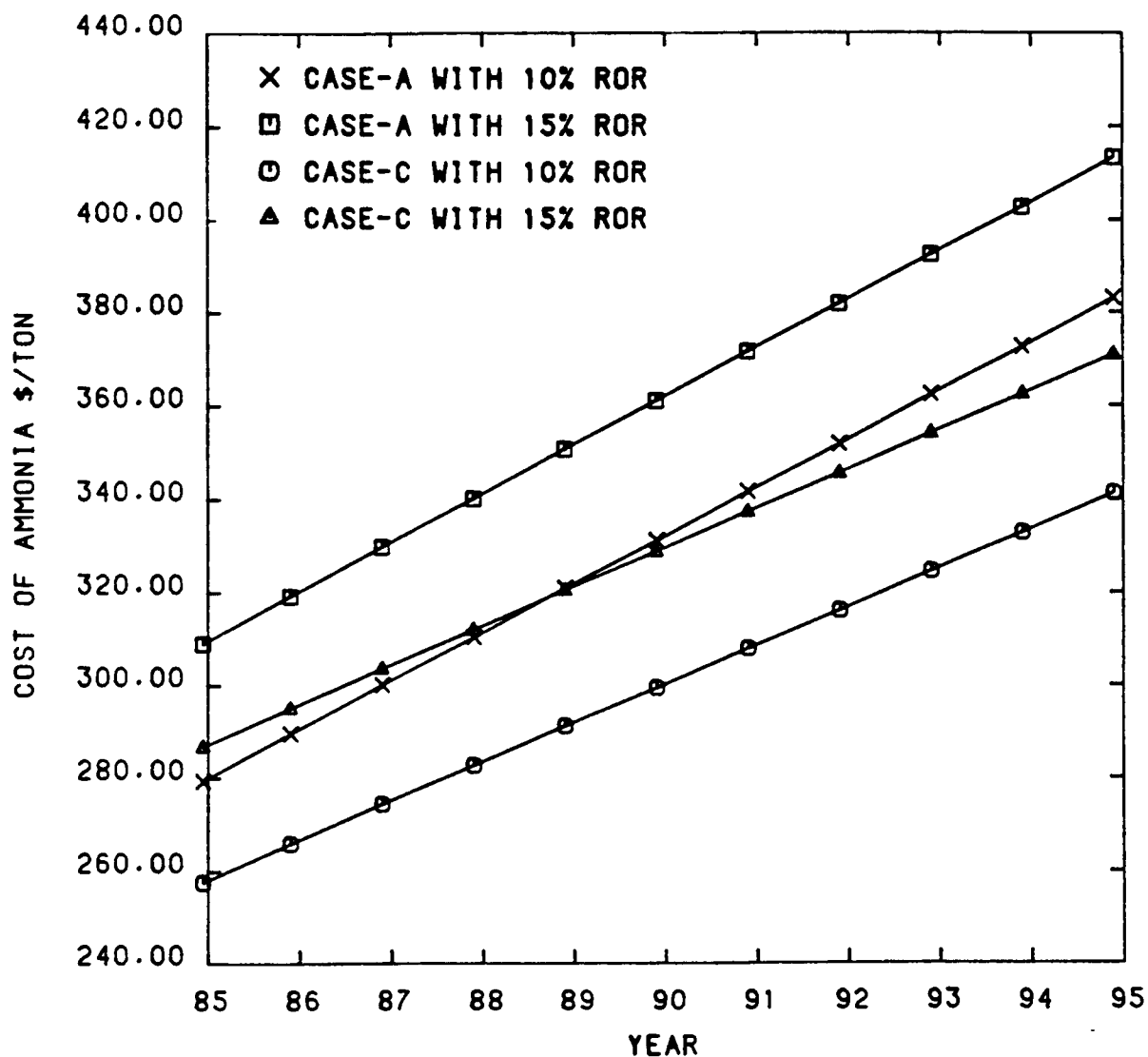


Figure 6.5. Ammonia cost comparison for Case A and Case C, DCF with SYD depreciation and 50 percent debt to equity ratio

TABLE 6.7

COST COMPARISON--CONVENTIONAL PROCESS AND AFBC ARRANGEMENT--DCF
WITH SYD DEPRECIATION AND 100 PERCENT DEBT TO EQUITY RATIO

Year	Cost of ammonia \$/ton (1983 dollars)			
	10% ROR		15% ROR	
	Case A	Case C	Case A	Case C
1985	285.05	263.20	309.96	287.61
1986	295.30	271.50	320.29	295.98
1987	305.87	280.01	330.94	304.56
1988	316.11	288.31	341.27	312.93
1989	326.68	296.82	351.92	321.50
1990	336.92	305.11	362.25	329.86
1991	347.49	313.62	372.90	338.43
1992	357.73	321.90	383.23	346.79
1993	368.30	330.41	393.88	355.36
1994	378.55	338.69	404.21	363.72
1995	389.11	347.18	414.86	372.27

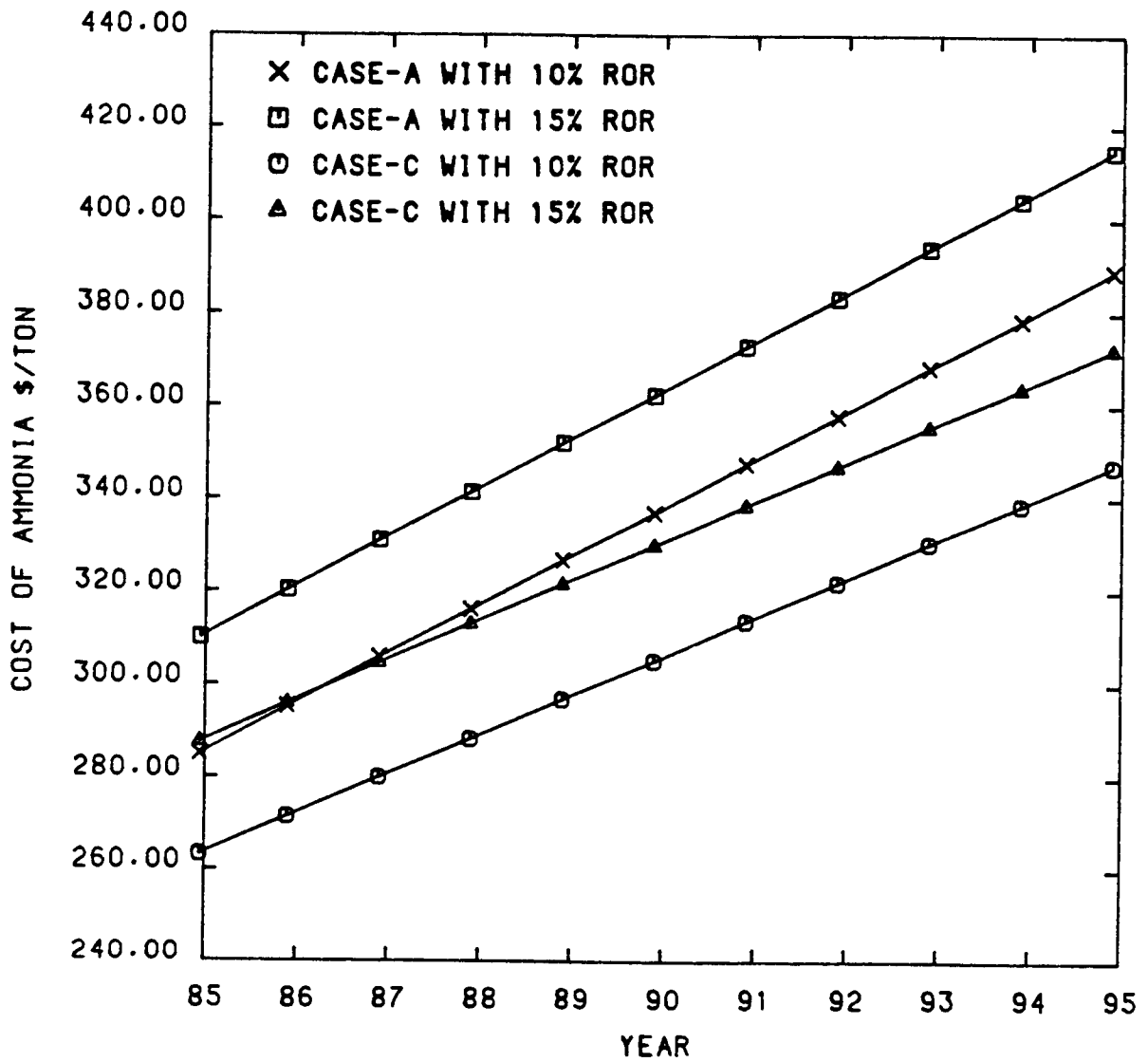


Figure 6.6. Ammonia cost comparison for Case A and Case C, DCF with SYD depreciation and 100 percent debt to equity ratio

TABLE 6.8

COST COMPARISON--CONVENTIONAL PROCESS AND AFBC ARRANGEMENT--DCF
WITH ACRS DEPRECIATION AND 50 PERCENT DEBT TO EQUITY RATIO

Year	Cost of ammonia \$/ton (1983 dollars)			
	10% ROR		15% ROR	
	Case A	Case C	Case A	Case C
1985	278.28	256.59	306.44	284.23
1986	288.49	264.86	316.71	292.56
1987	299.02	273.33	327.30	301.09
1988	309.23	281.61	337.58	309.41
1989	319.76	290.09	348.17	317.94
1990	329.97	298.34	358.44	326.25
1991	340.49	306.82	369.04	334.78
1992	350.70	315.08	379.31	343.09
1993	361.23	323.56	389.90	351.62
1994	371.44	331.81	400.19	359.92
1995	381.97	340.27	410.79	368.44

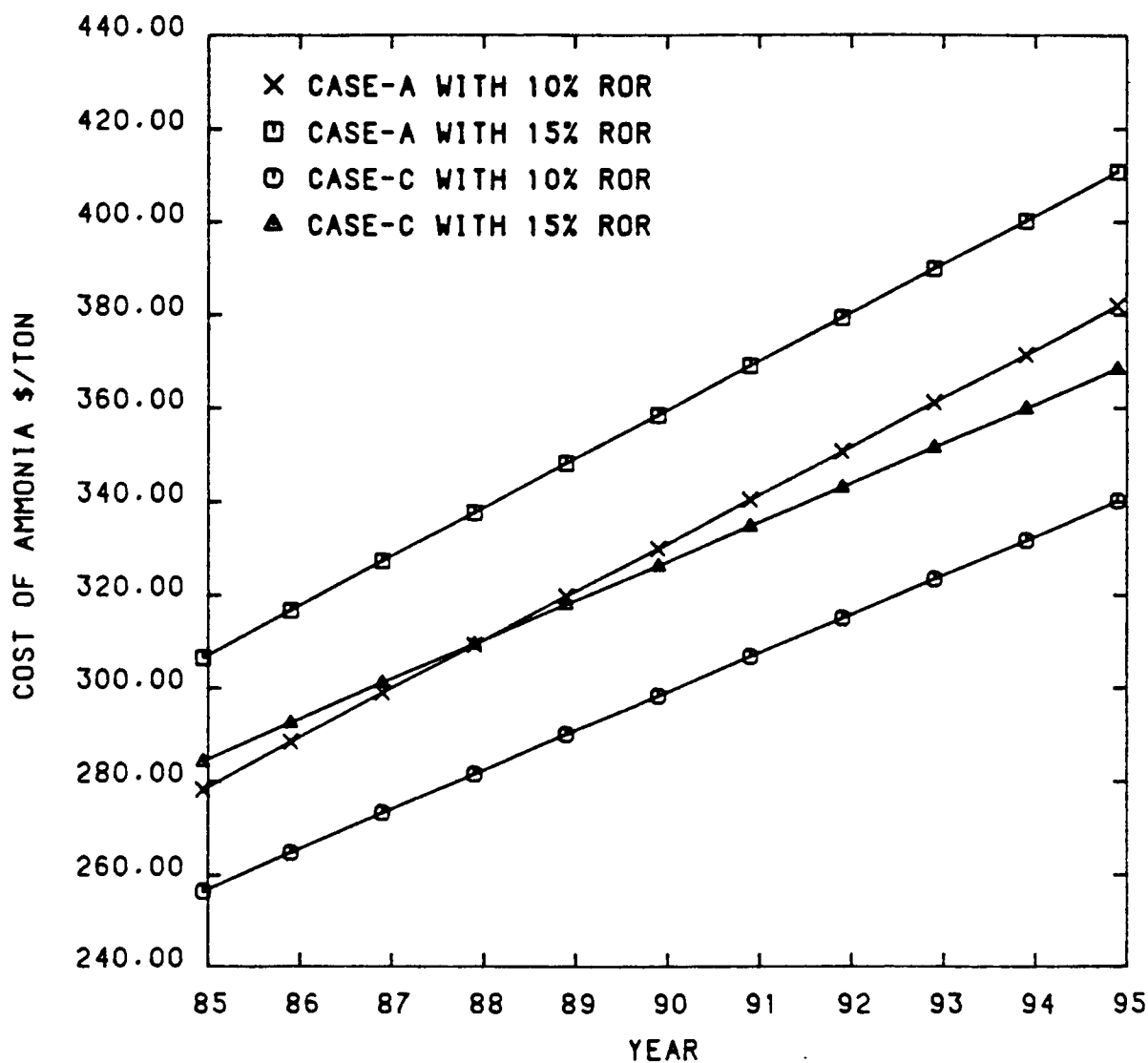


Figure 6.7. Ammonia cost comparison for Case A and Case C, DCF with ACRS depreciation and 50 percent debt to equity ratio

TABLE 6.9

COST COMPARISON--CONVENTIONAL PROCESS AND AFBC ARRANGEMENT--DCF
WITH ACRS DEPRECIATION AND 100 PERCENT DEBT TO EQUITY RATIO

Year	Cost of ammonia \$/ton (1983 dollars)			
	10% ROR		15% ROR	
	Case A	Case C	Case A	Case C
1985	283.65	261.84	307.39	285.11
1986	293.89	270.13	317.70	293.46
1987	304.44	278.63	328.33	302.02
1988	314.68	286.92	338.65	310.38
1989	325.24	295.42	349.28	318.94
1990	335.49	303.71	359.59	327.28
1991	346.05	312.20	370.23	335.84
1992	356.30	320.20	380.54	344.18
1993	366.87	328.99	391.17	352.74
1994	377.11	337.28	401.48	361.08
1995	387.68	345.77	412.12	369.63

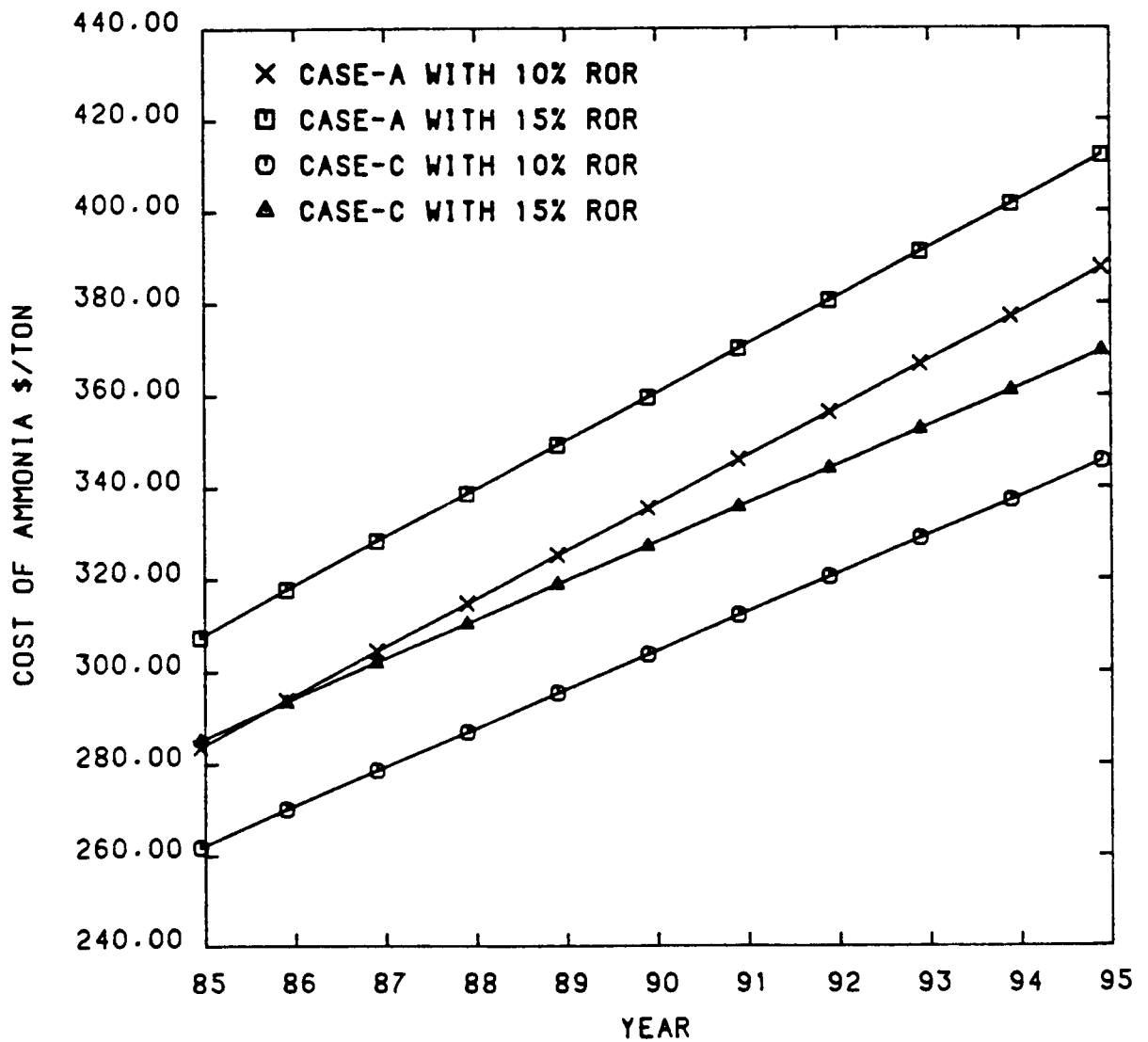


Figure 6.8. Ammonia cost comparison for Case A and Case C, DCF with ACRS depreciation and 100 percent debt to equity ratio

TABLE 6.10

COST COMPARISON--CONVENTIONAL PROCESS AND MBG ARRANGEMENT--DCF
WITH SYD DEPRECIATION AND 50 PERCENT DEBT TO EQUITY RATIO

Year	Cost of ammonia \$/ton (1983 dollars)			
	10% ROR		15% ROR	
	Case A	Case D	Case A	Case D
1985	279.35	298.26	308.90	341.74
1986	289.57	305.86	319.19	349.39
1987	300.10	313.64	329.79	357.23
1988	310.32	321.24	340.08	364.88
1989	320.86	329.02	350.69	372.72
1990	331.07	336.60	360.97	380.36
1991	341.61	344.39	371.58	388.26
1992	351.83	351.97	381.87	395.83
1993	362.36	359.75	392.47	403.67
1994	372.58	367.33	402.76	411.31
1995	383.12	375.10	413.37	419.13

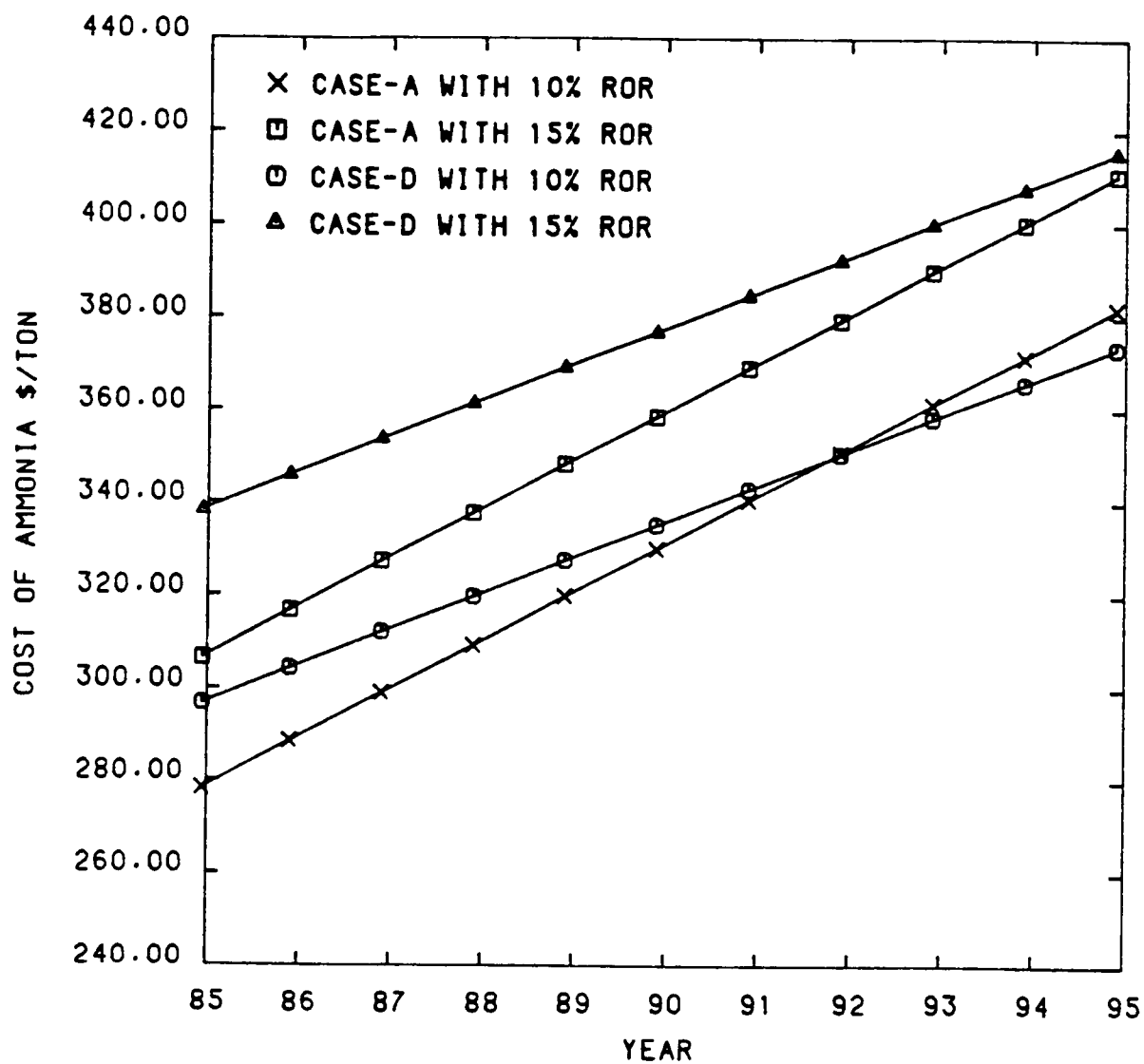


Figure 6.9. Ammonia cost comparison for Case A and Case D, DCF with SYD depreciation and 50 percent debt to equity ratio

It is observed that the costs for Case D are higher compared to Case A and this arrangement is apparently not economical. There is a break even point for the 10 percent rate of return, however it lies around the year 1992 while the 15 percent rate of return break even point is beyond 1995. The cost data for these two cases with 100 percent debt to equity ratio are presented in Table 6.11 and compared in Figure 6.10. It is found that the break even for the switch over is further shifted toward the year 1993. The change in depreciation method doesn't have a beneficial impact on the price of ammonia in this alternative arrangement also. The ammonia costs for the ACRS depreciation method are presented in Tables 6.12 and 6.13. These costs are compared in Figures 6.11 and 6.12. In both the cases (50 and 100 percent debt to equity ratio) the costs have shown a slight decrease compared to the previous depreciation method. Regarding the increase in debt ratio, the increase in cost for 10 percent ROR (rate of return) is slightly more than that of 15 percent ROR. However, the costs with 15 percent ROR for Case D do not show any break even point in time with the costs of Case A.

6.3 Summary for the analyses

From the above analysis, it is observed that the type of depreciation method does not affect the cost of ammonia to a great extent. An increase in the debt fraction of the investment shows a small effect on the cost, but not to a large degree. An increase in rate of return on equity shifted the break even in time in almost all the cases, indicating it's sensitivity on the cost of ammonia.

TABLE 6.11

COST COMPARISON--CONVENTIONAL PROCESS AND MBG ARRANGEMENT--DCF
WITH SYD DEPRECIATION AND 100 PERCENT DEBT TO EQUITY RATIO

Year	Cost of ammonia \$/ton (1983 dollars)			
	10% ROR		15% ROR	
	Case A	Case D	Case A	Case D
1985	285.05	306.48	309.96	342.85
1986	295.30	314.10	320.29	350.53
1987	305.87	321.90	330.94	358.41
1988	316.11	329.52	341.27	366.09
1989	326.68	337.33	351.92	373.97
1990	336.92	344.94	362.25	381.64
1991	347.49	352.74	372.90	389.52
1992	357.73	360.35	383.23	397.19
1993	368.30	368.16	393.88	405.06
1994	378.55	375.76	404.21	412.73
1995	389.11	383.55	414.86	420.59

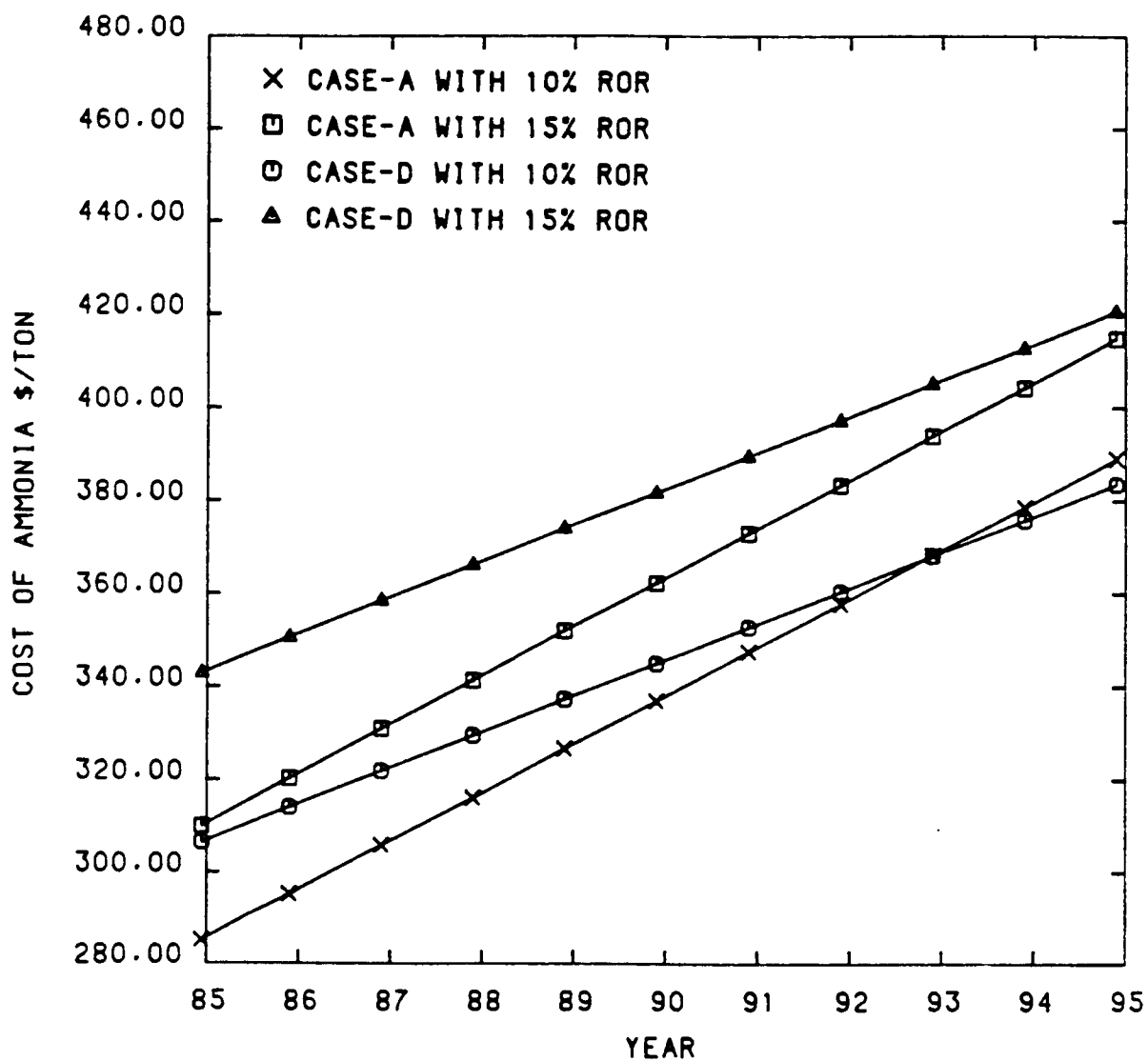


Figure 6.10. Ammonia cost comparison for Case A and Case D, DCF with SYD depreciation and 100 percent debt to equity ratio

TABLE 6.12

COST COMPARISON--CONVENTIONAL PROCESS AND MBG ARRANGEMENT--DCF
WITH ACRS DEPRECIATION AND 50 PERCENT DEBT TO EQUITY RATIO

Year	Cost of ammonia \$/ton (1983 dollars)			
	10% ROR		15% ROR	
	Case A	Case D	Case A	Case D
1985	278.28	296.74	306.44	338.20
1986	288.49	304.33	316.71	345.84
1987	299.02	312.11	327.30	353.66
1988	309.23	319.70	337.58	361.31
1989	319.76	327.48	348.17	369.14
1990	329.97	335.06	358.44	376.76
1991	340.49	342.83	369.04	384.59
1992	350.70	350.41	379.31	392.22
1993	361.23	358.19	389.90	400.05
1994	371.44	365.76	400.19	407.67
1995	381.97	373.52	410.79	415.49

TABLE 6.13

COST COMPARISON--CONVENTIONAL PROCESS AND MBG ARRANGEMENT--DCF
WITH ACRS DEPRECIATION AND 100 PERCENT DEBT TO EQUITY RATIO

Year	Cost of ammonia \$/ton (1983 dollars)			
	10% ROR		15% ROR	
	Case A	Case D	Case A	Case D
1985	283.65	304.48	307.39	339.19
1986	293.89	312.10	317.70	346.86
1987	304.44	319.89	328.33	354.72
1988	314.68	327.51	338.65	362.39
1989	325.24	335.31	349.28	370.26
1990	335.49	342.90	359.59	377.91
1991	346.05	350.70	370.23	385.77
1992	356.30	358.30	380.54	393.43
1993	366.87	366.10	391.17	401.29
1994	377.11	373.70	401.48	408.95
1995	387.68	381.48	412.12	416.79

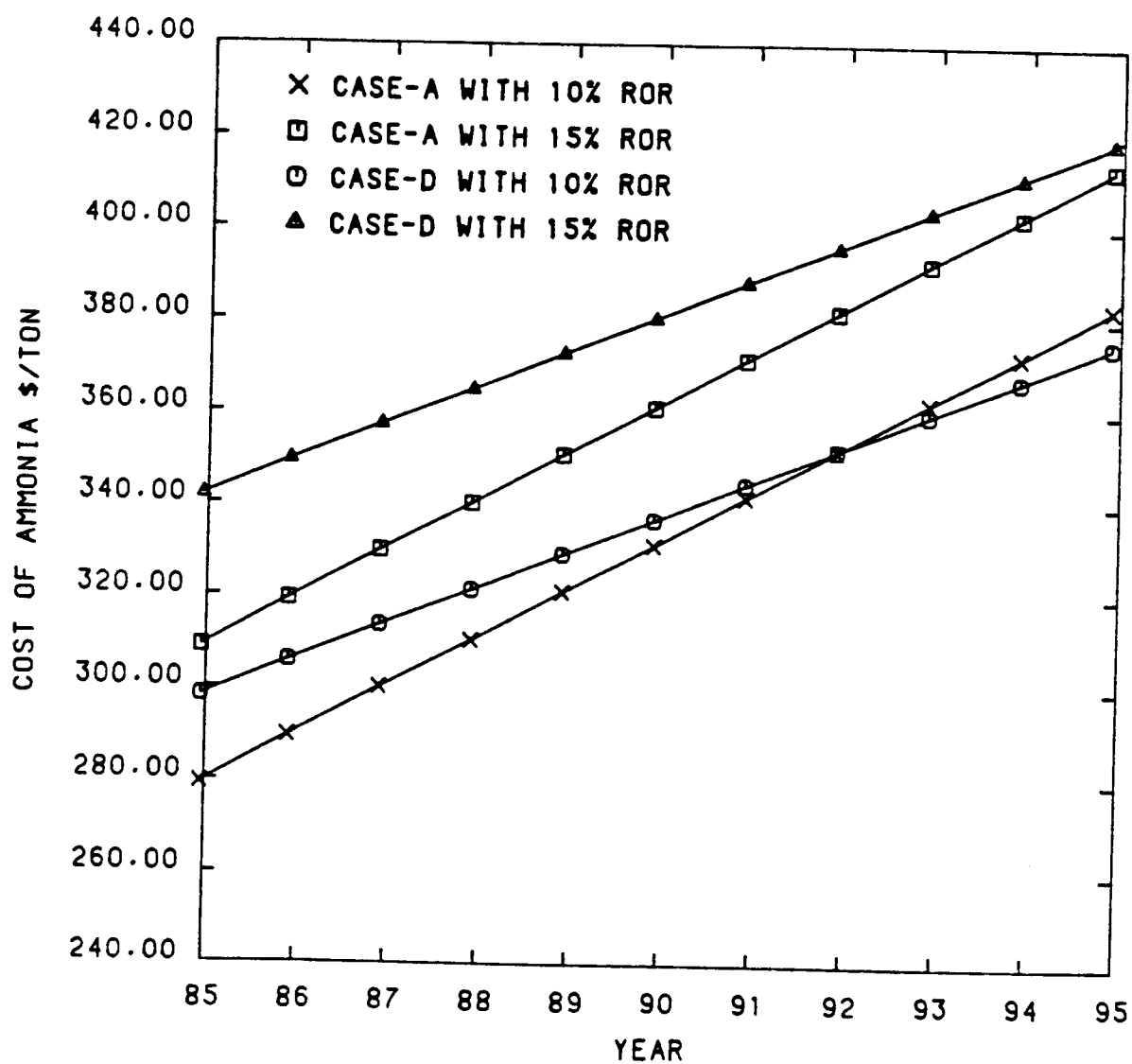


Figure 6.11. Ammonia cost comparison for Case A and Case D, DCF with ACRS depreciation and 50 percent debt to equity ratio

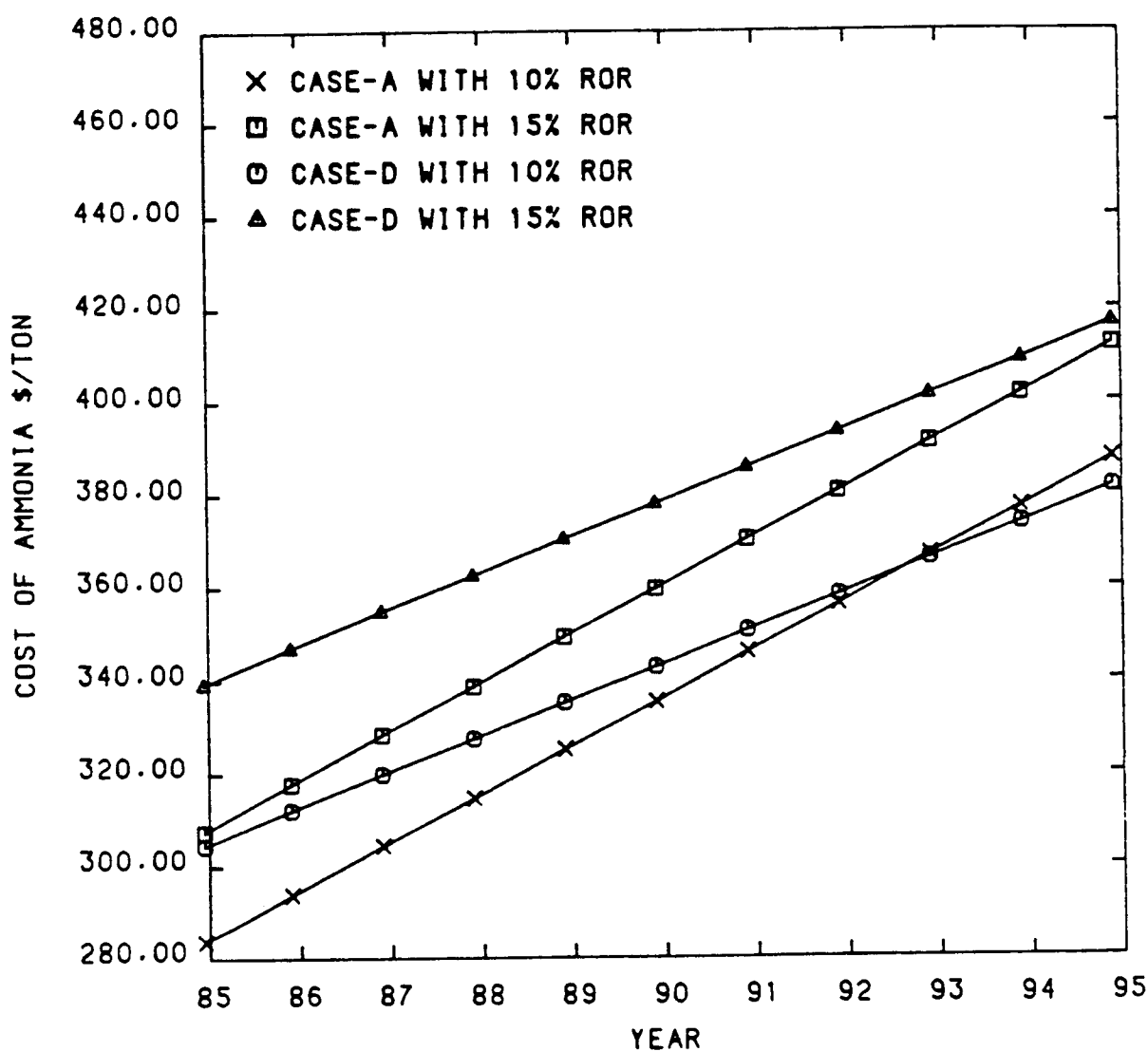


Figure 6.12. Ammonia cost comparison for Case A and Case D, DCF with ACRS depreciation and 100 percent debt to equity ratio

In general, it is found that the cost of ammonia is more sensitive to the price of natural gas compared to that of coal. This is indicated by the magnitude of increase in ammonia cost year by year. Apparently the non-conventional process (Case B) will be competitive with conventional plants by 1988-1989 assuming 10 percent rate of return on investment and by 1992 assuming 15 percent rate of return on investment. The AFBC arrangement (Case C) is found to be attractive for the future years. The MBG arrangement (Case D) is not found to be economic because of the higher investment involved in the MBG plant. However, at 10 percent rate of return on investment, the break even point with a conventional ammonia process (Case A) will probably occur by 1992. Some sulfur is produced in the MBG plant, however it is assumed that it will have no appreciable impact on the cost of ammonia. In the non-conventional process for manufacturing ammonia from coal (Case B), some sulfur is also produced for which a reasonable credit in the range of \$ 1 to \$ 3 per ton of ammonia would be given. However, in the present study this is not considered for the reasons of simplicity.

CHAPTER VII

CONCLUSIONS AND RECOMMENDATIONS

This study is made to develop possible alternatives to replace the expensive natural gas used for manufacturing the energy-based-chemical, ammonia. The alternative energy source, coal, has been considered to replace natural gas as fuel as well as feedstock. The mass and energy balances for the different flow sheets required for the various process alternatives are performed using the ASPEN computer program. It was found that ASPEN gave relatively quick and accurate balances both for the conventional and non-conventional process flow sheets. The results obtained from ASPEN simulations were found to be in reasonable agreement with the data reported in the literature. ASPEN was found to be highly flexible and capable of giving reasonably accurate results for various process engineering calculations.

An economic study is made for the following process alternatives.

Case A: Natural gas--Ammonia, a conventional process with natural gas as feed and fuel.

Case B: Coal--Ammonia, a non-conventional process with coal as the feed which is gasified in a Texaco gasifier.

Case C: Natural gas--AFBC--Ammonia, with natural gas as feed and a coal-fired AFBC reformer.

Case D: Natural gas--MBG--Ammonia, with natural gas as feed and medium BTU gas (MBG) as the fuel for reformer.

Case B considers an alternative process using coal as the only raw material for the ammonia process. Case C and Case D are considered to

evaluate the alternative arrangements for replacing the conventional natural gas-fired reformer furnace. The results from ASPEN simulations were utilized to develop the economics for the different processes.

The economics of manufacturing 1000 tons of ammonia per day with the conventional process and other alternative arrangements were developed utilizing discounted cash flow analysis with the help of CASHFLOW computer program. The production cost of ammonia (in 1983 dollars per ton) was considered as the economic criterion in all cases for the comparison of the different process alternatives. Forecasts of future ammonia prices were developed for each alternative and the years when the alternative product prices would become equal to or less than those for the conventional process were predicted. The effects of the type of depreciation method, the rate of return on equity and debt to equity ratio were studied through sensitivity analysis.

It is observed that the alternative arrangement AFBC (Case C) is economical and appears to be competitive with the conventional process right from the year 1985. It is found that coal as a feedstock (Case B) can compete with natural gas only after the years 1988 and 1992 with 10 percent and 15 percent rates of return (after taxes) respectively. The MBG arrangement (Case D) does not appear attractive in the near future.

In general, it is found that the type of depreciation does not have a significant impact on the cost of ammonia. However, the cost of ammonia appears to be sensitive to the rate of return on equity and the break even point in time for the change over to the alternative processes is shifted to later dates. It is also found

that an increase in investment debt affects the cost of ammonia but not to a great extent. Processes involving gasification of coal are highly capital intensive and their economics appear attractive only with cheaper financing methods (lower return on equity and interest rates). In this study, the interest rate on debt is considered as 9 percent assuming that a lower cost financing will be made available through Federal corporations like the Synfuel Corporation as an encouragement to new coal projects.

It was found that the cost of ammonia production is more sensitive to natural gas price factors than those for coal since natural gas prices are projected to increase more rapidly than coal prices. In this study, the future prices of natural gas and coal are projected to increase linearly at rates of 64 percent and 46 percent respectively, during the next 10 year period. Therefore those alternatives based upon coal feedstock will become more attractive with time due to lower relative raw material costs.

In the present study, the atmospheric fluidized bed combustor arrangement is found to be economically attractive. A special type of catalyst tube material will be required for this arrangement in order to permit heat transfer in the reformer at a low temperature approach. An in-depth study of special Nickel-Chromium alloys for the tube design material is recommended for further work. The basic concepts developed by the present work could be helpful for sizing and studying the arrangement of catalyst tubes for optimum heat transfer in the AFBC furnace. Exploring the possibility of using a pressurized fluidized bed combustor is another alternative that is recommended.

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LIST OF REFERENCES

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APPENDIXES

APPENDIX A-I

ASPEN CODE FOR CONVENTIONAL PROCESS
FLOWSHEET SIMULATION

```

//NATGS JOB ,DANTULURI,GROUP=J50251,USER=P89108,PASSWORD=,
//  TIME=3,MSGLEVEL=(2,1),MSGCLASS=H
/*JOBPARM ROOM=GRAD,LINES=99,FORMS=0216
/*ROUTE CMSRJO USERID=PA89108
/*ROUTE PRINT RMT1
/*SETUP STORCC
//PROCLIB DD DSN=J050251.ASPENRUN.PROCS,DISP=SHR
//STEP1 EXEC ASPEN,USER=J50251,RUNID=NATGS,REGION=1500K,
//  PRINT='*'
//RUN.SYSIN DD *
NEW
TITLE  'DESIGN OF  NATURAL GAS TO AMMONIA PLANT'
;
DESCRIPTION  "ASPEN SIMULATOR IS USED TO PERFORM A PRELIMINARY
            MATERIAL AND ENERGY BALANCES IN A PLANT PRODUCING AMMONIA
            FROM NATURAL GAS"
;
;
;*****
;
;          DESCRIPTION OF THE DESIGN BASIS
;
;
;*****
;
;THIS PLANT PRODUCES 1000 SHORT TONS OF AMMONIA PER DAY BY STEAM
;REFORMING PROCESS OF NATURAL GAS.THE PRIMARY REFORMER IS FIRED
;WITH NATURAL GAS.MATERIAL AND ENERGY BALANCES ARE BEING STUDIED
;TO REPLACE NATURAL GAS WITH ALTERNATIVE FUEL.
;
;
;
RUN-CONTROL MAX-TIME=200
;
IN-UNITS  MET  TEMPERATURE=C
OUT-UNITS  MET  TEMPERATURE=C
;
HISTORY MSG-LEVEL PROPERTIES=2
;
;
;*****
;
;          PHYSICAL PROPERTY DATA
;*****
;
COMPONENTS  AR AR / C2H6 C2H6 / H2 H2 / CO CO / CO2 CO2 / N2 N2 /
            O2 O2 / H2O H2O / H3N H3N / CH4 CH4 / C3H8 C3H8
PROPERTIES  SYSOP4 GLOBAL
;
;
;
COMP-NAMES  AR ARGON / C2H6 ETHANE / H2 HYDROGEN / CO CARBONMONOXIDE /
            CO2 CARBONDIOXIDE / N2 NITROGEN / O2 OXYGEN / H2O WATER /
            H3N AMMONIA / CH4 METHANE / C3H8 PROPANE
;
;
;
SC-COMPS    SCLIST1  H2  CH4  N2

```

```

;*****
;
;           FLOW SHEET
;
;*****
;
; FLOWSHEET
;
; REFORMING SECTION
;
; BLOCK  M201      IN=S201  S202 S203 S204 S205      OUT=S206
; BLOCK  H202      IN=S206
; BLOCK  M203      IN=S207  S208      OUT=S209
; BLOCK  R204      IN=S209
; BLOCK  M205      IN=S210  S211 S218      OUT=S212
; BLOCK  R206      IN=S212
; BLOCK  R207      IN=S213
; BLOCK  H208      IN=S214      OUT=S215
;
; SHIFT SECTION
;
; BLOCK  M301      IN=S215  S301      OUT=S302
; BLOCK  R302      IN=S302
; BLOCK  H302A     IN=S303
; BLOCK  R302B     IN=S304
; BLOCK  H303      IN=S304A
; BLOCK  E305      IN=S305      OUT=S308 S309
; BLOCK  R306      IN=S308
; BLOCK  HA306     IN=S310
; BLOCK  E307      IN=S311      OUT=S312 S313
;
;
; SYNTHESIS SECTION
;
; BLOCK  K401      IN=S312
; BLOCK  H401A     IN=S312A
; BLOCK  K401B     IN=S401A
; BLOCK  H401C     IN=S401B
; BLOCK  K401D     IN=S401C
; BLOCK  M402      IN=S401  S411
; BLOCK  R404      IN=S403
; BLOCK  H404A     IN=S404
; BLOCK  D405      IN=S405
; BLOCK  H406      IN=S406
; BLOCK  E408      IN=S407
;
; *****
;
;           STREAM DATA
;
; *****
;
; DEF-STREAMS  HEAT  Q1
;
; THE FEED STOCK I.E NATURAL GAS IS ASSUMED TO CONTAIN CH4-93.25%,
; C2H6-3.3%,N2-1.95%,AR-0.40%,C3H8-1.09%
;
; STREAM  S201

```

```

        SUBSTREAM    MIXED PRES=32    TEMP=150
        MOLE-FLOW    CH4    872.86
STREAM    S202
        SUBSTREAM    MIXED PRES=32    TEMP=150
        MOLE-FLOW    C2H6    30.8827
STREAM    S203
        SUBSTREAM    MIXED PRES=32    TEMP=150
        MOLE-FLOW    C3H8    10.21
STREAM    S204
        SUBSTREAM    MIXED PRES=32    TEMP=150
        MOLE-FLOW    N2     18.09
STREAM    S205
        SUBSTREAM    MIXED PRES=32    TEMP=150
        MOLE-FLOW    AR     3.705
STREAM    S208
        SUBSTREAM    MIXED PRES=35    TEMP=250
        MOLE-FLOW    H2O    1671.6
STREAM    S211
        SUBSTREAM    MIXED PRES=18    TEMP=80
        MOLE-FLOW    N2     1158.05
STREAM    S218
        SUBSTREAM    MIXED PRES=18    TEMP=80
        MOLE-FLOW    O2     40.28
STREAM    S301
        SUBSTREAM    MIXED PRES=18.0  TEMP=185
        MOLE-FLOW    H2O    808.6

```

```

;
;*****
;

```

UNIT OPERATIONS SPECIFICATIONS

```

;*****
;

```

;REFORMING SECTION

BLOCK M201 MIXER

;THE FEED IS PREHEATED

BLOCK H202 HEATER

DESCRIPTION 'FEED PREHEATER'

PARAM TEMP=400 PRES=-1.0

BLOCK M203 MIXER

;THE PROCESS STEAM IS MIXED WITH THE PREHEATED FEED AND SENT TO REFORMER

;THE REACTIONS ASSUMED TO OCCUR IN THE PRIMARY REFORMER ARE

; CH4+H2O----> CO+3H2; C2H6+4H2O---->7H2+2CO2

; C3H8+6H2O----->10H2+3CO2

BLOCK R204 RSTOIC

PARAM TEMP=770 PRES=16 NPK=1

STOI 1 MIXED CH4 -1 / H2O -1 / CO 1 / H2 3

STOI 2 MIXED C2H6 -1 / H2O -4 / H2 7 / CO2 2

STOI 3 MIXED C3H8 -1 / H2O -6 / H2 10 / CO2 3

CONV 1 MIXED CH4 0.60

CONV 2 MIXED C2H6 0.95

CONV 3 MIXED C3H8 0.95

```

;
;NITROGEN FOR SYNTHESIS IS FED TO SECONDARY REFORMER.ALSO SOME AIR IS

```

```

;IS SUPPLIED SO THAT SOME OF THE METHANE IS BURNED TO SUPPLY HEAT.
BLOCK  M205  MIXER
;UNREACTED METHANE IS ASSUMED TO BE CONVERTED IN SECONDARY REFORMER.
BLOCK  R206  RSTOIC
    PARAM  TEMP=770  PRES=16  NPK=1
    STOI  1  MIXED CH4  -1 / O2  -2 / CO2  .1 / H2O  2
    STOI  2  MIXED C2H6  -2 / O2  -7 / CO2  4 / H2O  6
    CONV  1  MIXED CH4  0.20
    CONV  2  MIXED C2H6  0.95
BLOCK  R207  RSTOIC
    PARAM  TEMP=770  PRES=16.0  NPK=1
    STOI  1  MIXED CH4  -1 / H2O  -1 / H2  3 / CO  1
    CONV  1  MIXED CH4  0.95
;
; HEAT IS EXTRACTED FROM HOT GASES
BLOCK  H208  HEATER
    PARAM  TEMP=360  PRES=-5
;SHIFT SECTION
BLOCK  M301  MIXER
; STEAM REQUIRED FOR SHIFT REACTION IS MIXED HERE
    PARAM  PRES=-0.1
BLOCK  R302  RSTOIC
; THIS IS HIGH TEMP SHIFT REACTOR WHEREIN THE REACTION CO+H2O -->CO2+H2
; TAKESPLACE.THE CONVERSION OF CO IS ASSUMED TO BE 98%
    PARAM  TEMP=425
    STOI  1  MIXED CO  -1 / H2O  -1 / CO2  1 / H2  1
    CONV  1  MIXED CO  0.50
BLOCK  H302A  HEATER
    PARAM  TEMP=215  PRES=-2.0
;THIS IS THE LOW TEMP SHIFT REACTOR
BLOCK  R302B  RSTOIC
    PARAM  TEMP=215
    STOI  1  MIXED CO  -1 /H2O  -1 / CO2  1/ H2  1
    CONV  1  MIXED CO  0.97
;
BLOCK  H303  HEATER
; THIS IS THE HEAT EXCHANGER TO COOL THE SHIFTED PRODUCTS
;
    PARAM  TEMP=130  PRES=-2.0
;
;
BLOCK  E305  SEP2
; THIS IS TO REMOVE CARBONDIOXIDE BY MEA PROCESS.IT IS ASSUMED THAT
; 99% OF CO2 IS REMOVED BY THIS PROCESS.
    FLASH-SPECS  S308  TEMP=300  PRES=21  NPK=1  KPH=1/
                    S309  TEMP=65  PRES=21  NPK=1  KPH=1
    FRAC SUBS=MIXED STRM=S308 COMP=H2 CH4 CO CO2 N2 O2 C3H8 H2O C2H6 AR &
    FRAC=.999 .999 .999 .01 .999 .999 .999 .999 .999 .999 /
    STRM=S309 COMP=H2 CH4 CO CO2 N2 O2 C3H8 H2O C2H6 AR &
    FRAC=.001 .001 .001 .99 .001 .001 .001 .001 .001 .001
BLOCK  R306  REQUIL
;
; THIS IS METHANATOR FOR FINAL PURIFICATION OF SYNTHESIS GAS
;THE REACTIONS INVOLVED ARE 3H2+CO--->CH4+H2O ; 4H2+CO2--->CH4+2H2O

```

```

PARAM NR=2    TEMP=310  PRES=21  NPK=1
STOI  1  H2  -3 0 / CO  -1 0 / CH4  1 0 / H2O  1 0
STOI  2  H2  -4 0 / CO2  -1 0 / CH4  1 0 / H2O  2 0
;
BLOCK HA306    HEATER
; THIS IS TO COOL METHANATOR OUTLETS
PARAM  TEMP=200  PRES=-1.0
BLOCK E307  SEP2
; THIS IS TO SEPARATE METHANE BEFORE COMPRESSING SYNTHESIS GAS
FLASH-SPECS  S312    TEMP=30    PRES=20    NPK=1    KPH=1/
                S313    TEMP=200    PRES=3
FRAC SUBS=MIXED STRM=S312 COMP=H2 CH4 CO CO2 N2 O2 C3H8 H2O AR C2H6 &
FRAC=.999 .01 .0005 .0005 .999 .0005 .0005 .0005 .0005 .0005 /
STRM=S313 COMP=H2 CH4 CO CO2 N2 O2 C3H8 H2O AR C2H6 &
FRAC=.001 .99 .9995 .9995 .001 .9995 .9995 .9995 .9995 .9995
;
;
BLOCK K401  COMPR
; THE GAS MIXTURE IS COMPRESSED TO 300 ATM.
PARAM  1  100  TEMP=250
BLOCK H401A HEATER
PARAM  TEMP=50
BLOCK K401B COMPR
PARAM  1  200  TEMP=125
BLOCK H401C HEATER
PARAM  TEMP=50
BLOCK K401D COMPR
PARAM  1  300  TEMP=300
BLOCK M402  MIXER
PARAM  PRES=-0.1
BLOCK R404  RSTOIC
; THIS IS THE SYNTHESIS REACTOR
PARAM  TEMP=450 PRES=300
STOICH  1  MIXED  H2  -3 / N2  -1 / H3N  2
CONV  1  MIXED  H2  0.40
BLOCK H404A HEATER
PARAM  TEMP=305  PRES=-10
;
BLOCK D405  SEP2
; THIS IS TO SEPARATE UNREACTED GASES FROM AMMONIA
FLASH-SPECS  S406    TEMP=50  PRES=4    NPK=1    KPH=1/
                S407    TEMP=300  PRES=275  NPK=1    KPH=1
FRAC SUBS=MIXED STRM=S406 COMP=H3N H2 CH4 N2 O2 CO CO2 C3H8 H2O AR &
FRAC=.999 .0005 .0005 .0005 .0005 .0 .0 .0 .0 .001 /
STRM=S407 COMP=H3N H2 CH4 N2 O2 CO CO2 C3H8 H2O AR &
FRAC=.001 .9995 .9995 .9995 .9995 1.0 1.0 1.0 1.0 0.999
;
BLOCK H406  HEATER
; THIS IS TO COOL THE AMMONIA VAPORS
PARAM  TEMP=-33.3  PRES=-1.5
;
BLOCK E408  FSPLIT
;THIS IS TO PURGE SOME OF THE RECYCLE.
;

```

```
FRAC S411 0.96/ S412 0.04
;
;
SIMULATE
;
REPORT STREAMS BLOCKS FLOWSHEET
//FORT.SYSPRINT DD DUMMY
//LKED.SYSPRINT DD DUMMY
//STEP2 EXEC ASPPURGE,USER=J50251,RUNID=NATGS
```

APPENDIX A-II

STREAM DATA FROM ASPEN FOR
CONVENTIONAL PROCESS

DESIGN OF NATURAL GAS TO AMMONIA PLANT
STREAM SECTION

=====

S203 S204 S205 S208 S211

STREAM ID	S203	S204	S205	S208	S211
FROM :					
TO :	M201	M201	M201	M203	M205
CLASS:	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL				
AR	KMOL/HR	0.0	0.0	3.7050	0.0	0.0
C2H6	KMOL/HR	0.0	0.0	0.0	0.0	0.0
H2	KMOL/HR	0.0	0.0	0.0	0.0	0.0
CO	KMOL/HR	0.0	0.0	0.0	0.0	0.0
CO2	KMOL/HR	0.0	0.0	0.0	0.0	0.0
N2	KMOL/HR	0.0	18.0900	0.0	0.0	1158.0500
O2	KMOL/HR	0.0	0.0	0.0	0.0	0.0
H2O	KMOL/HR	0.0	0.0	0.0	1671.6000	0.0
H3N	KMOL/HR	0.0	0.0	0.0	0.0	0.0
CH4	KMOL/HR	0.0	0.0	0.0	0.0	0.0
C3H8	KMOL/HR	10.2100	0.0	0.0	0.0	0.0
TOTAL	KMOL/HR	10.2100	18.0900	3.7050	1671.6000	1158.0500
TEMP	C	150.0000	150.0000	150.0000	250.0000	80.0000
PRES	ATM	32.0000	32.0000	32.0000	35.0000	18.0000
ENTHALPY	CAL/MOL	-.22810+05	854.2247	587.8430	-.56352+05	362.8362
VFRAC		1.0000	1.0000	1.0000	1.0000	1.0000
LFRAC		0.0	0.0	0.0	0.0	0.0
ENTROPY	CAL/MOL-K	-65.0970	-4.5039	-5.2225	-13.5687	-4.6227
DENSITY	MOL/CC	0.0011	.91125-03	.92060-03	.93704-03	.61948-03
AVG MW		44.0970	28.0130	39.9480	18.0150	28.0130

DESIGN OF NATURAL GAS TO AMMONIA PLANT
STREAM SECTION

=====

S206 S207 S209 S210 S212

STREAM ID	S206	S207	S209	S210	S212
FROM :	M201	H202	M203	R204	M205
TO :	H202	M203	R204	M205	R206
CLASS:	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN

SUBSTREAM: MIXED	STRUCTURE: CONVENTIONAL				
AR KMOL/HR	3.7050	3.7050	3.7050	3.7050	3.7050
C2H6 KMOL/HR	30.8827	30.8827	30.8827	1.5441	1.5441
H2 KMOL/HR	0.0	0.0	0.0	1873.5130	1873.5130
CO KMOL/HR	0.0	0.0	0.0	523.7160	523.7160
CO2 KMOL/HR	0.0	0.0	0.0	87.7756	87.7756
N2 KMOL/HR	18.0900	18.0900	18.0900	18.0900	1176.1400
O2 KMOL/HR	0.0	0.0	0.0	0.0	40.2800
H2O KMOL/HR	0.0	0.0	1671.6000	972.3327	972.3327
H3N KMOL/HR	0.0	0.0	0.0	0.0	0.0
CH4 KMOL/HR	872.8600	872.8600	872.8600	349.1440	349.1440
C3H8 KMOL/HR	10.2100	10.2100	10.2100	0.5105	0.5105
TOTAL KMOL/HR	935.7477	935.7477	2607.3477	3830.3310	5028.6610
TEMP C	149.5111	400.0000	310.1659	770.0000	629.8745
PRES ATM	32.0000	31.0000	31.0000	16.0000	16.0000
ENTHALPY CAL/MOL	-.16516+05-	.13411+05-	.40941+05-	.15933+05-	.12050+05
VFRAC	1.0000	1.0000	1.0000	1.0000	1.0000
LFRAC	0.0	0.0	0.0	0.0	0.0
ENTROPY CAL/MOL-K	-23.1088	-17.3321	-13.4091	5.6728	5.0401
DENSITY MOL/CC	.93573-03	.55719-03	.67442-03	.18645-03	.21525-03
AVG MW	17.1380	17.1380	17.7002	12.0488	15.8849

DESIGN OF NATURAL GAS TO AMMONIA PLANT
STREAM SECTION

=====

S213 S214 S215 S302 S303

STREAM ID	S213	S214	S215	S302	S303
FROM :	R206	R207	H208	M301	R302
TO :	R207	H208	M301	R302	H302A
CLASS:	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL				
AR	KMOL/HR	3.7050	3.7050	3.7050	3.7050	3.7050
C2H6	KMOL/HR	1.1360	1.1360	1.1360	1.1360	1.1360
H2	KMOL/HR	1873.5130	2813.2097	2813.2097	2813.2097	3231.6838
CO	KMOL/HR	523.7160	836.9482	836.9482	836.9482	418.4741
CO2	KMOL/HR	108.0176	108.0176	108.0176	108.0176	526.4917
N2	KMOL/HR	1176.1400	1176.1400	1176.1400	1176.1400	1176.1400
O2	KMOL/HR	0.0	0.0	0.0	0.0	0.0
H2O	KMOL/HR	1012.4087	699.1764	699.1764	1507.7764	1089.3023
H3N	KMOL/HR	0.0	0.0	0.0	0.0	0.0
CH4	KMOL/HR	329.7181	16.4859	16.4859	16.4859	16.4859
C3H8	KMOL/HR	0.5105	0.5105	0.5105	0.5105	0.5105
TOTAL	KMOL/HR	5028.8650	5655.3295	5655.3295	6463.9295	6463.9295
TEMP	C	770.0000	770.0000	360.0000	186.3244	425.0000
PRES	ATM	16.0000	16.0000	11.0000	10.9000	10.9000
ENTHALPY	CAL/MOL	- .11595+05	-7315.7626	- .10487+05	- .17371+05	- .16146+05
VFRAC		1.0000	1.0000	1.0000	1.0000	1.0000
LFRAC		0.0	0.0	0.0	0.0	0.0
ENTROPY	CAL/MOL-K	6.2399	8.1862	5.0813	1.3309	3.9311
DENSITY	MOL/CC	.18635-03	.18632-03	.21124-03	.28994-03	.18994-03
AVG MW		15.8843	14.1247	14.1247	14.6114	14.6114

DESIGN OF NATURAL GAS TO AMMONIA PLANT
STREAM SECTION

=====

S304 S304A S305 S308 S309

STREAM ID	S304	S304A	S305	S308	S309
FROM :	H302A	R302B	H303	E305	E305
TO :	R302B	H303	E305	R306	
CLASS:	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL				
AR	KMOL/HR	3.7050	3.7050	3.7050	3.7012	0.0037
C2H6	KMOL/HR	1.1360	1.1360	1.1360	1.1349	0.0011
H2	KMOL/HR	3231.6838	3637.6037	3637.6037	3633.9661	3.6376
CO	KMOL/HR	418.4741	12.5542	12.5542	12.5416	0.0125
CO2	KMOL/HR	526.4917	932.4116	932.4116	9.3241	923.0875
N2	KMOL/HR	1176.1400	1176.1400	1176.1400	1174.9639	1.1761
O2	KMOL/HR	0.0	0.0	0.0	0.0	0.0
H2O	KMOL/HR	1089.3023	683.3824	683.3824	682.6990	0.6833
H3N	KMOL/HR	0.0	0.0	0.0	0.0	0.0
CH4	KMOL/HR	16.4859	16.4859	16.4859	16.4694	0.0164
C3H8	KMOL/HR	0.5105	0.5105	0.5105	0.5099	.51050-03
TOTAL	KMOL/HR	6463.9295	6463.9295	6463.9295	5535.3104	928.6190
TEMP	C	215.0000	215.0000	130.0000	300.0000	65.0000
PRES	ATM	8.9000	8.9000	6.9000	21.0000	21.0000
ENTHALPY	CAL/MOL	-.17770+05	-.18368+05	-.19014+05	-5452.3431	-.93350+05
VFRAC		1.0000	1.0000	1.0000	1.0000	1.0000
LFRAC		0.0	0.0	0.0	0.0	0.0
ENTROPY	CAL/MOL-K	1.5692	0.6303	-0.3180	-0.9312	-4.5061
DENSITY	MOL/CC	.22232-03	.22214-03	.20888-03	.44487-03	.82219-03
AVG MW		14.6114	14.6115	14.6115	9.7139	43.8053

DESIGN OF NATURAL GAS TO AMMONIA PLANT
STREAM SECTION

=====

S310 SA310 S311 S312 S313

STREAM ID	S310	SA310	S311	S312	S313
FROM :	R306	R306	HA306	E307	E307
TO :	HA306		E307	K401	
CLASS:	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL				
AR	KMOL/HR	3.7012	0.0	3.7012	0.0018	3.6994
C2H6	KMOL/HR	1.1349	0.0	1.1349	.56746-03	1.1343
H2	KMOL/HR	3559.0446	0.0	3559.0446	3555.4856	3.5590
CO	KMOL/HR	.53466-08	0.0	.53466-08	.26733-11	.53439-08
CO2	KMOL/HR	.35357-07	0.0	.35357-07	.17678-10	.35339-07
N2	KMOL/HR	1174.9639	0.0	1174.9639	1173.7889	1.1749
O2	KMOL/HR	0.0	0.0	0.0	0.0	0.0
H2O	KMOL/HR	713.8889	0.0	713.8889	0.3569	713.5320
H3N	KMOL/HR	0.0	0.0	0.0	0.0	0.0
CH4	KMOL/HR	38.3352	0.0	38.3352	0.3833	37.9518
C3H8	KMOL/HR	0.5099	0.0	0.5099	.25499-03	0.5097
TOTAL	KMOL/HR	5491.5788	0.0	5491.5788	4730.0174	761.5613
TEMP	C	310.0000	MISSING	200.0000	30.0000	200.0000
PRES	ATM	21.0000	21.0000	20.0000	20.0000	3.0000
ENTHALPY	CAL/MOL	-5613.2452	MISSING	-6415.8281	21.4486-	.53683+05
VFRAC		1.0000	MISSING	1.0000	1.0000	1.0000
LFRAC		0.0	MISSING	0.0	0.0	0.0
ENTROPY	CAL/MOL-K	-0.9804	MISSING	-2.4080	-4.7539	-8.8512
DENSITY	MOL/CC	.43728-03	MISSING	.51424-03	.80007-03	.78246-04
AVG MW		9.7912	MISSING	9.7912	8.4697	17.9993

DESIGN OF NATURAL GAS TO AMMONIA PLANT
STREAM SECTION

=====

S312A S401A S401B S401C S401

STREAM ID	S312A	S401A	S401B	S401C	S401
FROM :	K401	H401A	K401B	H401C	K401D
TO :	H401A	K401B	H401C	K401D	M402
CLASS:	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL				
AR	KMOL/HR	0.0018	0.0018	0.0018	0.0018	0.0018
C2H6	KMOL/HR	.56746-03	.56746-03	.56746-03	.56746-03	.56746-03
H2	KMOL/HR	3555.4856	3555.4856	3555.4856	3555.4856	3555.4856
CO	KMOL/HR	.26733-11	.26733-11	.26733-11	.26733-11	.26733-11
CO2	KMOL/HR	.17678-10	.17678-10	.17678-10	.17678-10	.17678-10
N2	KMOL/HR	1173.7889	1173.7889	1173.7889	1173.7889	1173.7889
O2	KMOL/HR	0.0	0.0	0.0	0.0	0.0
H2O	KMOL/HR	0.3569	0.3569	0.3569	0.3569	0.3569
H3N	KMOL/HR	0.0	0.0	0.0	0.0	0.0
CH4	KMOL/HR	0.3833	0.3833	0.3833	0.3833	0.3833
C3H8	KMOL/HR	.25499-03	.25499-03	.25499-03	.25499-03	.25499-03
TOTAL	KMOL/HR	4730.0174	4730.0174	4730.0174	4730.0174	4730.0174
TEMP	C	250.0000	50.0000	125.0000	50.0000	300.0000
PRES	ATM	100.000	100.000	200.0000	200.0000	300.0000
ENTHALPY	CAL/MOL	1565.3086	145.1993	684.2058	141.1777	1968.5158
VFRAC		1.0000	1.0000	1.0000	1.0000	1.0000
LFRAC		0.0	0.0	0.0	0.0	0.0
ENTROPY	CAL/MOL-K	-4.1821	-7.6027	-7.5554	-9.0668	-5.7607
DENSITY	MOL/CC	0.0022	0.0036	0.0056	0.0069	0.0057
AVG MW		8.4697	8.4697	8.4697	8.4697	8.4697

DESIGN OF NATURAL GAS TO AMMONIA PLANT
STREAM SECTION

=====

S403 S404 S405 S406 S407

STREAM ID	S403	S404	S405	S406	S407
FROM :	M402	R404	H404A	D405	D405
TO :	R404	H404A	D405	H406	E408
CLASS:	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL				
AR	KMOL/HR	0.0450	0.0450	0.0450	.45094-04	0.0450
C2H6	KMOL/HR	0.0141	0.0141	0.0141	0.0	0.0141
H2	KMOL/HR	8379.8872	5027.9323	5027.9323	2.5139	5025.4183
CO	KMOL/HR	.26733-11	0.0	0.0	0.0	0.0
CO2	KMOL/HR	.17678-10	0.0	0.0	0.0	0.0
N2	KMOL/HR	2513.1425	1395.8242	1395.8242	0.6979	1395.1263
O2	KMOL/HR	0.0	0.0	0.0	0.0	0.0
H2O	KMOL/HR	8.9031	8.9031	8.9031	0.0	8.9031
H3N	KMOL/HR	2.1473	2236.7839	2236.7839	2234.5471	2.2367
CH4	KMOL/HR	9.4502	9.4502	9.4502	0.0047	9.4454
C3H8	KMOL/HR	0.0063	0.0063	0.0063	0.0	0.0063
TOTAL	KMOL/HR	.10914+05	8678.9593	8678.9593	2237.7638	6441.1956
TEMP	C	300.3811	450.0000	305.0000	50.0000	300.0000
PRES	ATM	274.9000	300.0000	290.0000	4.0000	275.0000
ENTHALPY	CAL/MOL	1905.8604	405.9271	-849.8693	-.10739+05	1858.1289
VFRAC		1.0000	1.0000	1.0000	1.0000	1.0000
LFRAC		0.0	0.0	0.0	0.0	0.0
ENTROPY	CAL/MOL-K	-5.6171	-8.8336	-10.6992	-25.7824	-5.6581
DENSITY	MOL/CC	0.0053	0.0047	0.0057	.15505-03	0.0053
AVG MW		8.0308	10.0987	10.0987	17.0175	7.6950

DESIGN OF NATURAL GAS TO AMMONIA PLANT
STREAM SECTION

=====

S408 S411 S412 S201 S202

STREAM ID	S408	S411	S412	S201	S202
FROM :	H406	E408	E408		
TO :		M402		M201	M201
CLASS:	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL				
AR	KMOL/HR	.45094-04	0.0432	0.0018	0.0	0.0
C2H6	KMOL/HR	0.0	0.0135	.56615-03	0.0	30.8827
H2	KMOL/HR	2.5139	4824.4016	201.0167	0.0	0.0
CO	KMOL/HR	0.0	0.0	0.0	0.0	0.0
CO2	KMOL/HR	0.0	0.0	0.0	0.0	0.0
N2	KMOL/HR	0.6979	1339.3212	55.8050	0.0	0.0
O2	KMOL/HR	0.0	0.0	0.0	0.0	0.0
H2O	KMOL/HR	0.0	8.5470	0.3561	0.0	0.0
H3N	KMOL/HR	2234.5471	2.1473	0.0894	0.0	0.0
CH4	KMOL/HR	0.0047	9.0676	0.3778	872.8600	0.0
C3H8	KMOL/HR	0.0	0.0061	.25441-03	0.0	0.0
TOTAL	KMOL/HR	2237.7638	6183.5478	257.6478	872.8600	30.8827
TEMP	C	-33.3000	300.0000	300.0000	150.0000	150.0000
PRES	ATM	2.5000	275.0000	275.0000	32.0000	32.0000
ENTHALPY	CAL/MOL	-.17028+05	1858.1289	1858.1289	-.16798+05	-.18697+05
VFRAC		0.0022	1.0000	1.0000	1.0000	1.0000
LFRAC		0.9977	0.0	0.0	0.0	0.0
ENTROPY	CAL/MOL-K	-48.9443	-5.6581	-5.6581	-23.0348	-43.7902
DENSITY	MOL/CC	0.0182	0.0053	0.0053	.93281-03	0.0010
AVG MW		17.0175	7.6950	7.6950	16.0430	30.0700

DESIGN OF NATURAL GAS TO AMMONIA PLANT
STREAM SECTION

S218 S301

STREAM ID	S218	S301
FROM :		
TO :	M205	M301
CLASS:	CONVEN	CONVEN

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL	
AR	KMOL/HR	0.0	0.0
C2H6	KMOL/HR	0.0	0.0
H2	KMOL/HR	0.0	0.0
CO	KMOL/HR	0.0	0.0
CO2	KMOL/HR	0.0	0.0
N2	KMOL/HR	0.0	0.0
O2	KMOL/HR	40.2800	0.0
H2O	KMOL/HR	0.0	808.6000
H3N	KMOL/HR	0.0	0.0
CH4	KMOL/HR	0.0	0.0
C3H8	KMOL/HR	0.0	0.0
TOTAL	KMOL/HR	40.2800	808.6000
TEMP	C	80.0000	185.0000
PRES	ATM	18.0000	18.0000
ENTHALPY	CAL/MOL	359.2069-	.65518+05
VFRAC		1.0000	0.0
LFRAC		0.0	1.0000
ENTROPY	CAL/MOL-K	-4.6167	-31.4598
DENSITY	MOL/CC	.62425-03	0.0402
AVG MW		31.9990	18.0150

APPENDIX A-III

ASPEN CODE FOR STEAM BALANCE FLOWSHEET
SIMULATION IN CONVENTIONAL PROCESS

```

//STEAM JOB ,DANTULURI,GROUP=J50251,USER=P89108,PASSWORD=,
//    TIME=3,MSGLEVEL=(2,1),MSGCLASS=H
/*JOBPARM ROOM=GRAD,LINES=99
/*ROUTE CMSRJO USERID=PA89108
/*ROUTE PRINT RMT1
/*SETUP STORCC
//PROCLIB DD DSN=J050251.ASPENRUN.PROCS,DISP=SHR
//STEP1 EXEC ASPEN,USER=J50251,RUNID=STEAM,REGION=1500K,
//    PRINT='*'
//RUN.SYSIN DD *
NEW
TITLE 'STEAM BALANCE FOR NG-NH3 FLOW SHEET'
DESCRIPTION "ASPEN SIMULATOR IS USED TO PERFORM STEAM BALANCES"
RUN-CONTROL MAX-TIME=200
HISTORY MSG-LEVEL PROPERTIES=2
COMPONENTS H2O H2O
COMP-NAMES H2O WATER
PROPERTIES SYSOP5 SEC1 / SYSOP12 STEAMSEC
FLowsHEET SEC1
    BLOCK H101 IN=S101 OUT=S102
    BLOCK P103 IN=S102 OUT=S104
    BLOCK M104 IN=S104 S107A S111A OUT=S104A
    BLOCK H105 IN=S104A OUT=S105
FLowsHEET STEAMSEC
    BLOCK H200 IN=S105 OUT=S105A
    BLOCK F201 IN=S105A OUT=S106 S107
    BLOCK P201A IN=S107 OUT=S107A
    BLOCK F202 IN=S106 OUT=S108 S109
    BLOCK H202A IN=S109 OUT=S109A
    BLOCK F203 IN=S109A OUT=S110 S111
    BLOCK P203A IN=S111 OUT=S111A
CONVERGENCE STM WEGSTEIN
    TEAR S104A
SEQUENCE FLOW H101 P103 STM H105 H200 F201 F202 H202A F203 P203A P201A &
    M104 (RETURN STM)
DEF-STREAMS CONVEN SEC1/CONVEN STEAMSEC
STREAM S101
    SUBSTREAM MIXED TEMP=70 PRES=60 V-FRAC=0 FLASH-OPTION=1-PHASE
    MASS-FLOW H2O 95750
STREAM S102
    SUBSTREAM MIXED V-FRAC=0 FLASH-OPTION=1-PHASE
STREAM S104
    SUBSTREAM MIXED V-FRAC=0 FLASH-OPTION=1-PHASE
STREAM S104A
    SUBSTREAM MIXED TEMP=344.46 PRES=1500
    MOLE-FLOW H2O 11973
STREAM S105
    SUBSTREAM MIXED TEMP=600 PRES=1500 FLASH-OPTION=1-PHASE
STREAM S106
    SUBSTREAM MIXED V-FRAC=1.0 FLASH-OPTION=1-PHASE
STREAM S107
    SUBSTREAM MIXED FLASH-OPTION=1-PHASE
STREAM S107A

```

```

      SUBSTREAM MIXED V-FRAC=0 FLASH-OPTION=1-PHASE
STREAM S110
      SUBSTREAM MIXED V-FRAC=1.0 FLASH-OPTION=1-PHASE
STREAM S111A
      SUBSTREAM MIXED V-FRAC=0 FLASH-OPTION=1-PHASE
STREAM S111
      SUBSTREAM MIXED V-FRAC=0 FLASH-OPTION=1-PHASE
BLOCK H101 HEATER
      PARAM TEMP=190 PRES=-10.0
BLOCK P103 PUMP
      PARAM PRES=1500 TYPE=1 EFF=0.6
BLOCK M104 MIXER
;STEAM COIL
BLOCK H105 HEATER
      PARAM TEMP=600
;SUPER HEATING COIL
BLOCK H200 HEATER
      PARAM TEMP=900
BLOCK F201 FLASH2
;TURBINE FOR SYN COMPRESSORS
      PARAM TEMP=480 DUTY=-75.68D+06
BLOCK P201A PUMP
      PARAM PRES=1500 TYPE=1 EFF=0.6
BLOCK F202 FSPLIT
      FRAC S109 0.403/ S108 0.597
;SUPERHEATING
BLOCK H202A HEATER
      PARAM TEMP=750
;TURBINE FOR POWER GENERATION
BLOCK F203 FLASH2
      PARAM TEMP=420 DUTY=-20.32D+06
BLOCK P203A PUMP
      PARAM PRES=1500 TYPE=1 EFF=0.6
SIMULATE
//FORT.SYSPRINT DD DUMMY
//LKED.SYSPRINT DD DUMMY
//STEP2 EXEC ASPPURGE,USER=J50251,RUNID=STEAM

```

APPENDIX A-IV

STREAM DATA FROM ASPEN FOR STEAM
BALANCE IN CONVENTIONAL PROCESS

STEAM BALANCE FOR NG-NH3 FLOW SHEET
STREAM SECTION

=====

S102 S104 S104A S105 S101

STREAM ID	S102	S104	S104A	S105	S101
FROM :	H101	P103	M104	H105	
TO :	P103	M104	H105	H200	H101
CLASS:	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL				
H2O	LBMOL/HR	5315.0153	5315.0153	9079.9491	9079.9491	5315.0153
TOTAL	LBMOL/HR	5315.0153	5315.0153	9079.9491	9079.9491	5315.0153
TEMP	F	190.0000	193.7947	305.2697	600.0000	70.0000
PRES	PSI	50.0000	1500.0000	1500.0000	1500.0000	60.0000
ENTHALPY	BTU/LBMOL	-.12199+06	-.12185+06	-.11924+06	-.10161+06	-.12451+06
VFRAC		0.0	0.0	0.0	1.0000	0.0
LFRAC		1.0000	1.0000	1.0000	0.0	1.0000
ENTROPY	BTU/LBMOL-R	-37.2211	-37.1350	-33.4529	-15.5116	-41.4835
DENSITY	LBMOL/CUFT	3.1855	3.1829	2.9745	0.1772	3.4203
AVG MW		18.0150	18.0150	18.0150	18.0150	18.0150

STEAM BALANCE FOR NG-NH3 FLOW SHEET
STREAM SECTION

=====

S105A S106 S107 S107A S108

STREAM ID	S105A	S106	S107	S107A	S108
FROM :	H200	F201	F201	P201A	F202
TO :	F201	F202	P201A	M104	
CLASS:	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL				
H2O	LBMOL/HR	9079.9491	6163.4180	2916.5311	2916.5311	3679.5605
TOTAL	LBMOL/HR	9079.9491	6163.4180	2916.5311	2916.5311	3679.5605
TEMP	F	900.0000	480.0000	480.0000	484.9818	480.0000
PRES	PSI	1500.0000	566.1507	566.1507	1500.0000	566.1507
ENTHALPY	BTU/LBMOL	-.98021+05-	.10208+06-	.11540+06-	.11529+06-	.10208+06
VFRAC		1.0000	1.0000	0.0	0.0	1.0000
LFRAC		0.0	0.0	1.0000	1.0000	0.0
ENTROPY	BTU/LBMOL-R	-12.4913	-14.3889	-28.5653	-28.5215	-14.3889
DENSITY	LBMOL/CUFT	0.1134	0.0679	2.7750	2.7859	0.0679
AVG MW		18.0150	18.0150	18.0150	18.0150	18.0150

STEAM BALANCE FOR NG-NH3 FLOW SHEET
STREAM SECTION

=====

S109 S109A S110 S111 S111A

STREAM ID	S109	S109A	S110	S111	S111A
FROM :	F202	H202A	F203	F203	P203A
TO :	H202A	F203		P203A	M104
CLASS:	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL				
H2O	LBMOL/HR	2483.8574	2483.8574	1636.1772	847.6802	847.6802
TOTAL	LBMOL/HR	2483.8574	2483.8574	1636.1772	847.6802	847.6802
TEMP	F	480.0000	750.0000	420.0000	420.0000	425.3551
PRES	PSI	566.1507	566.1507	308.7796	308.7796	1500.0000
ENTHALPY	BTU/LBMOL	-.10208+06-	.98870+05-	.10209+06-	.11662+06-	.11649+06
VFRAC		1.0000	1.0000	1.0000	0.0	0.0
LFRAC		0.0	0.0	0.0	1.0000	1.0000
ENTROPY	BTU/LBMOL-R	-14.3889	-11.3598	-13.3779	-29.8855	-29.8292
DENSITY	LBMOL/CUFT	0.0679	0.0461	0.0370	2.9315	2.9427
AVG MW		18.0150	18.0150	18.0150	18.0150	18.0150

APPENDIX B-I

ASPEN CODE FOR NON-CONVENTIONAL PROCESS
FLOWSHEET SIMULATION

```

//TEXCO JOB ,DANTULURI,GROUP=J50251,USER=P89108,PASSWORD=,
//      TIME=3,MSGLEVEL=(2,1),MSGCLASS=H
/*JOBPARM  ROOM=GRAD,LINES=99,FORMS=0216
/*ROUTE CMSRJO  USERID=PA89108
/*ROUTE PRINT RMT1
/*SETUP  STORCC
//PROCLIB DD  DSN=J050251.ASPENRUN.PROCS,DISP=SHR
//STEP1 EXEC ASPEN,USER=J50251,RUNID=TEXCO,REGION=1500K,
//      PRINT='*'
//RUN.SYSIN DD *
NEW
TITLE  'DESIGN OF COAL TO AMMONIA PLANT'
;
DESCRIPTION  "ASPEN SIMULATOR IS USED TO PERFORM A PRELIMINARY
              MATERIAL AND ENERGY BALANCES IN A PLANT PRODUCING AMMONIA
              FROM COAL"
;
;
;*****
;
;          DESCRIPTION OF THE DESIGN BASIS
;
;
;*****
;
;  THIS PLANT PRODUCING AMMONIA FROM COAL IS LOCATED IN
;MIDWEST AREA.THE PLANT HAS A CAPACITY OF 1000 SHORT TONS PER DAY.
;THE PLANT EMPLOYS TEXACO GASIFIER FOR COAL GASIFICATION.
;
;
;
RUN-CONTROL MAX-TIME=200
;
IN-UNITS  MET  TEMPERATURE=C
OUT-UNITS  MET  TEMPERATURE=C
;
HISTORY MSG-LEVEL PROPERTIES=2
;
;
;*****
;
;          PHYSICAL PROPERTY DATA
;
;*****
;
COMPONENTS  COAL / ASH / H2 H2 / CO CO / CO2 CO2 / N2 N2 / O2 O2 /
            H2O H2O / H3N H3N / CH4 CH4 / H2S H2S
PROPERTIES  SYSOP4 GLOBAL
;
ATTR-COMPS  COAL  ULTANAL PROXANAL / ASH PROXANAL
;
COMP-NAMES  COAL COAL / ASH ASH / H2 HYDROGEN / CO CARBONMONOXIDE /
            CO2 CARBONDIOXIDE / N2 NITROGEN / O2 OXYGEN / H2O WATER /
            H3N AMMONIA / CH4 METHANE / H2S HYDROGENSULFIDE
;
NC-PROPS  COAL  ENTHALPY  H2C1BOIE 1 / DENSITY DCOALIGT

```

```

;
SC-COMPS  SCLIST1  H2  CH4  N2
;
;*****
;
;          FLOW SHEET
;
;*****
;
; FLOWSHEET  SEC1
; FLOWSHEET OF NONCONVENTIONAL MATERIALS SECTION
;
; BLOCK  M101          IN=S101  S102          OUT=S103
; BLOCK  P102          IN=S103                OUT=S104
; BLOCK  H103          IN=S104                OUT=S105
; BLOCK  M104          IN=S105  S106          OUT=S107
; BLOCK  R105          IN=S107                OUT=S108
;
;
; FLOWSHEET  SEC2
; FLOWSHEET OF CONVENTIONAL MATERIALS SECTION
;
; GASIFICATION SECTION
;
; BLOCK  CLCHA          IN=S108                OUT=S201
; BLOCK  R201          IN=S201                OUT=S202  S203
; BLOCK  H202          IN=S202                OUT=S204
; BLOCK  M204          IN=S204  S207          OUT=S208
;
; SHIFT SECTION
;
; BLOCK  M301          IN=S208  S301          OUT=S302
; BLOCK  R302          IN=S302                OUT=S303
; BLOCK  H303          IN=S303                OUT=S305
; BLOCK  E305          IN=S305                OUT=S308  S309
; BLOCK  H306          IN=S309                OUT=S310
;
; SYNTHESIS SECTION
;
; BLOCK  K401          IN=S308                OUT=S401
; BLOCK  K401A          IN=S401                OUT=S401A
; BLOCK  M402          IN=S401A  S410          OUT=S402
; BLOCK  R404          IN=S402                OUT=S404
; BLOCK  H404A          IN=S404                OUT=S404A
; BLOCK  D405          IN=S404A                OUT=S406  S407
; BLOCK  H406          IN=S406                OUT=S409  Q1
; BLOCK  D407          IN=S407                OUT=S410  S411
;*****
;
;          STREAM DATA
;
;*****
;
; DEF-STREAMS MIXNC SEC1 / CONVEN SEC2
;
; DEF-STREAMS HEAT Q1
;
; STREAM  S101

```

```

SUBSTREAM NC PRES=1 TEMP=30
MASS-FLOW COAL 51250.0
;THE COAL UTILISED IS ILLINOIS NO.6 COAL
COMP-ATTR COAL ULTANAL (9.7 66.3 4.8 1.2 0 3.9 11.1)/
PROXANAL (10.2 46.0 34.7 9.1)
;
STREAM S102
SUBSTREAM MIXED PRES=1 TEMP=30
MOLE-FLOW H2O 2330.0
;
STREAM S106
SUBSTREAM MIXED PRES=70.0 TEMP=160
MOLE-FLOW O2 1690.0
;
STREAM S207
SUBSTREAM MIXED PRES=48.0 TEMP=500
MOLE-FLOW N2 1125.0
;
STREAM S301
SUBSTREAM MIXED PRES=48.0 TEMP=265
MOLE-FLOW H2O 980.7
;
STREAM S402
SUBSTREAM MIXED PRES=274.9 TEMP=300.2469
MOLE-FLOW H2 8273.9723 / CO 5.0001 / CO2 690.6536 /N2 2150.615 /
O2 10.7083 /H2O 23.8760 /H3N 2.121
;*****
;
UNIT OPERATIONS SPECIFICATIONS
;*****
;
BLOCK M101 MIXER
;CRUSHED COAL IS MIXED WITH WATER TO FORM SLURRY.
BLOCK P102 PUMP
DESCRIPTION 'COAL-WATER SLURRY PUMP'
PARAM PRES=25 TYPE=2
;
BLOCK H103 HEATER
DESCRIPTION 'PREHEATER FOR COAL-WATER SLURRY'
PARAM TEMP=160 PRES=-2
;
BLOCK M104 MIXER
PARAM PRES=-0.1
;
BLOCK R105 RSTOIC
;THE COMBUSTION SECTION OF THE GASIFIER IS MODELLED ASSUMING THAT
;COAL COMBUSTION FIRST TAKES PLACE IN AN IMAGINARY REACTOR WHEREIN
;ALL THE CARBON IN THE COAL IS CONVERTED TO CARBONMONOXIDE,WHICH
;FURTHER REACTS TO FORM CARBONDIOXIDE WITH THE EXCESS OXYGEN.AN
;OVERALL CONVERSION OF 99% WITH CHAR RECYCLE IS ASSUMED.THE RATIO
;FIGURES INDICATED BELOW ARE ON 10.00KG BASIS.
;
PARAM TEMP=1316 PRES=58.8

```

```

      STOICH  1  NC COAL -10.0 / MIXED O2 -0.3160 /
                MIXED CO 0.4731 / MIXED CO2 0.07938 / MIXED H2 0.2278 /
                MIXED H2S 0.012188 / MIXED N2 0.004286
      CONV  1  NC COAL 0.99
;
BLOCK  CLCHA  CLCHNG
;
BLOCK  R201  REQUIL
;
;THE PRODUCTS FROM THE ABOVE REACTOR ARE ASSUMED TO REACT AS FOLLOWING
;
;      CO+H2O  ----->  CO2 +H2
;
;      CO+3H2  ----->  CH4+H2O
;
      PARAM    NR=2  TEMP=1316  PRES=58.8  NPK=1
      STOI  1  CO -1 0 / H2O -1 0 / CO2 1 0 / H2 1 0
      STOI  2  CO -1 0 / H2 -3 0 / CH4 1 0 / H2O 1 0
;
BLOCK  H202  HEATER
; THIS IS A WASTE HEAT BOILER USED TO RECOVER HEAT FROM RAW GAS
      PARAM  TEMP=500  PRES=-3.0
BLOCK  M204  MIXER
; NITROGEN FROM AIR SEPARATION PLANT IS MIXED WITH THE RAW GAS
      PARAM  PRES=-0.1
BLOCK  M301  MIXER
; STEAM REQUIRED FOR SHIFT REACTION IS MIXED HERE
      PARAM  PRES=-0.1
BLOCK  R302  RSTOIC
; THIS IS SHIFT REACTOR WHEREIN THE REACTION CO+H2O -->CO2+H2
; TAKESPLACE.THE CONVERSION OF CO IS ASSUMED TO BE 98%
      PARAM  TEMP=425  PRES=50
      STOICH  1  MIXED CO -1 / H2O -1 / CO2 1 / H2 1
      CONV  1  MIXED CO 0.98
;
BLOCK  H303  HEATER
; THIS IS THE HEAT EXCHANGER TO COOL THE SHIFTED PRODUCTS
;
      PARAM  TEMP=80  PRES=-5.0
;
;
BLOCK  E305  SEP2
; THIS IS TO REMOVE ACID GAS AND CO2 BY RECTISOL PROCESS.IT'S ASSUMED
; 99% OF CO2 IS REMOVED BY THIS PROCESS.
      FLASH-SPECS  S308  TEMP=30  PRES=45  NPK=1  KPH=1/
                    S309  TEMP=30  PRES=21  NPK=1  KPH=1
      FRAC SUBS=MIXED STRM=S308 COMP=H2 CH4 CO CO2 N2 O2 H2S H2O &
                    FRAC=.999 .001 .005 .01 .999 .005 .0005 .001 /
                    STRM=S309 COMP=H2 CH4 CO CO2 N2 O2 H2S H2O &
                    FRAC=.001 .999 .995 .99 .001 .995 .9995 .999
BLOCK  H306  HEATER
      PARAM  TEMP=-25
;SYN GAS COMPRESSION SECTION
BLOCK  K401  COMPR
      PARAM  1  200  TEMP=250  EP=0.72
BLOCK  K401A  COMPR

```

```

PARAM 1 300 TEMP=300 EP=0.72
BLOCK M402 MIXER
PARAM PRES=-0.1
BLOCK R404 RSTOIC
; THIS IS THE SYNTHESIS REACTOR
PARAM TEMP=450 PRES=300
STOICH 1 MIXED H2 -3 / N2 -1 / H3N 2
CONV 1 MIXED H2 0.40
;
BLOCK H404A HEATER
PARAM TEMP=300
BLOCK D405 SEP2
; THIS IS TO SEPARATE UNREACTED GASES FROM AMMONIA
FLASH-SPECS S406 TEMP=30 PRES=3 NPK=1 KPH=1/
S407 TEMP=300 PRES=275 NPK=1 KPH=1
FRAC SUBS=MIXED STRM=S406 COMP=H3N H2 CH4 N2 O2 CO CO2 H2S H2O &
FRAC=.999 .0005 .0005 .0005 .0005 .000 .000 .000 .000 /
STRM=S407 COMP=H3N H2 CH4 N2 O2 CO CO2 H2S H2O &
FRAC=.001 .9995 .9995 .9995 .9995 1.0 1.0 1.0 1.0
;
BLOCK H406 HEATER
; THIS IS TO COOL THE AMMONIA VAPORS
PARAM TEMP=-33.3 PRES=-1.5
;
BLOCK D407 FSPLIT
;THIS IS TO PURGE SOME OF THE RECYCLE
FRAC S410 0.96 / S411 0.04

SIMULATE
;
REPORT STREAMS BLOCKS FLOWSHEET
//FORT.SYSPRINT DD DUMMY
//LKED.SYSPRINT DD DUMMY
//STEP2 EXEC ASPPURGE,USER=J50251,RUNID=TEXCO

```

APPENDIX B-II

STREAM DATA FROM ASPEN FOR
NON-CONVENTIONAL PROCESS

DESIGN OF COAL TO AMMONIA PLANT
STREAM SECTION

=====

S103 S104 S105 S107 S108

STREAM ID	S103	S104	S105	S107	S108
FROM :	M101	P102	H103	M104	R105
TO :	P102	H103	M104	R105	CLCHA
CLASS:	MIXNC	MIXNC	MIXNC	MIXNC	MIXNC

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL				
H2	KMOL/HR	0.0	0.0	0.0	0.0	1155.8002
CO	KMOL/HR	0.0	0.0	0.0	0.0	2400.3911
CO2	KMOL/HR	0.0	0.0	0.0	0.0	402.7542
N2	KMOL/HR	0.0	0.0	0.0	0.0	21.7460
O2	KMOL/HR	0.0	0.0	0.0	1690.0000	86.6950
H2O	KMOL/HR	2330.0000	2330.0000	2330.0000	2330.0000	2330.0000
H3N	KMOL/HR	0.0	0.0	0.0	0.0	0.0
CH4	KMOL/HR	0.0	0.0	0.0	0.0	0.0
H2S	KMOL/HR	0.0	0.0	0.0	0.0	61.8388
TOTAL	KMOL/HR	2330.0000	2330.0000	2330.0000	4020.0000	6459.2256
TEMP	C	30.0000	30.3545	160.0000	130.0250	1316.0000
PRES	ATM	1.0000	25.0000	23.0000	22.9000	58.8000
ENTHALPY	CAL/MOL	-.68624+05-	.68607+05-	.66042+05-	.37766+05-	.25384+05
VFRAC		0.0	0.0	0.0	0.4795	1.0000
LFRAC		1.0000	1.0000	1.0000	0.5204	0.0
ENTROPY	CAL/MOL-K	-39.6844	-39.6700	-32.6436	-19.9992	12.7977
DENSITY	MOL/CC	0.0469	0.0469	0.0416	0.0017	.44699-03
AVG MW		18.0150	18.0150	18.0150	23.8938	20.8625

SUBSTREAM: NC		STRUCTURE: NON CONVENTIONAL				
COAL	KG/HR	.51250+05	.51250+05	.51250+05	.51250+05	512.5000
ASH	KG/HR	0.0	0.0	0.0	0.0	0.0
TOTAL	KG/HR	.51250+05	.51250+05	.51250+05	.51250+05	512.5000
TEMP	C	30.0000	30.3545	160.0000	130.0250	1316.0000
PRES	ATM	1.0000	25.0000	23.0000	22.9000	58.8000
ENTHALPY	CAL/GM	-407.7969	-407.6923	-365.4366	-375.9270	431.4980
VFRAC		0.0	0.0	0.0	0.0	0.0
LFRAC		0.0	0.0	0.0	0.0	0.0
DENSITY	GM/CC	1.4576	1.4576	1.4576	1.4576	1.4576
AVG MW		1.0000	1.0000	1.0000	1.0000	1.0000
COMPONENT ATTRIBUTES:						
COAL	ULTANAL					
ASH		9.7000	9.7000	9.7000	9.7000	9.7000
CARBON		66.3000	66.3000	66.3000	66.3000	66.3000
HYDROGEN		4.8000	4.8000	4.8000	4.8000	4.8000
NITROGEN		1.2000	1.2000	1.2000	1.2000	1.2000
CHLORINE		0.0	0.0	0.0	0.0	0.0
SULFUR		3.9000	3.9000	3.9000	3.9000	3.9000
OXYGEN		11.1000	11.1000	11.1000	11.1000	11.1000
	PROXANAL					
MOISTURE		10.2000	10.2000	10.2000	10.2000	10.2000
FC		46.0000	46.0000	46.0000	46.0000	46.0000
VM		34.7000	34.7000	34.7000	34.7000	34.7000
ASH		9.1000	9.1000	9.1000	9.1000	9.1000

DESIGN OF COAL TO AMMONIA PLANT
STREAM SECTION

S101 S102 S106

STREAM ID	S101	S102	S106
FROM :			
TO :	M101	M101	M104
CLASS:	MIXNC	MIXNC	MIXNC

SUBSTREAM: MIXED

STRUCTURE: CONVENTIONAL

H2	KMOL/HR	0.0	0.0	0.0
CO	KMOL/HR	0.0	0.0	0.0
CO2	KMOL/HR	0.0	0.0	0.0
N2	KMOL/HR	0.0	0.0	0.0
O2	KMOL/HR	0.0	0.0	1690.0000
H2O	KMOL/HR	0.0	2330.0000	0.0
H3N	KMOL/HR	0.0	0.0	0.0
CH4	KMOL/HR	0.0	0.0	0.0
H2S	KMOL/HR	0.0	0.0	0.0
TOTAL	KMOL/HR	0.0	2330.0000	1690.0000
TEMP	C	MISSING	30.0000	160.0000
PRES	ATM	MISSING	1.0000	70.0000
ENTHALPY	CAL/MOL	MISSING	-.68624+05	900.6480
VFRAC		MISSING	0.0	1.0000
LFRAC		MISSING	1.0000	0.0
ENTROPY	CAL/MOL-K	MISSING	-39.6844	-5.9295
DENSITY	MOL/CC	MISSING	0.0469	0.0019
AVG MW		MISSING	18.0150	31.9990

SUBSTREAM: NC		STRUCTURE: NON CONVENTIONAL		
COAL	KG/HR	.51250+05	0.0	0.0
ASH	KG/HR	0.0	0.0	0.0
TOTAL	KG/HR	.51250+05	0.0	0.0
TEMP	C	30.0000	MISSING	MISSING
PRES	ATM	1.0000	MISSING	MISSING
ENTHALPY	CAL/GM	-407.7969	MISSING	MISSING
VFRAC		0.0	MISSING	MISSING
LFRAC		0.0	MISSING	MISSING
DENSITY	GM/CC	1.4576	MISSING	MISSING
AVG MW		1.0000	1.0000	1.0000
COMPONENT ATTRIBUTES:				
COAL	ULTANAL			
ASH		9.7000	MISSING	MISSING
CARBON		66.3000	MISSING	MISSING
HYDROGEN		4.8000	MISSING	MISSING
NITROGEN		1.2000	MISSING	MISSING
CHLORINE		0.0	MISSING	MISSING
SULFUR		3.9000	MISSING	MISSING
OXYGEN		11.1000	MISSING	MISSING
	PROXANAL			
MOISTURE		10.2000	MISSING	MISSING
FC		46.0000	MISSING	MISSING
VM		34.7000	MISSING	MISSING
ASH		9.1000	MISSING	MISSING

DESIGN OF COAL TO AMMONIA PLANT
STREAM SECTION

S201 S202 S203 S204 S208

STREAM ID	S201	S202	S203	S204	S208
FROM :	CLCHA	R201	R201	H202	M204
TO :	R201	H202		M204	M301
CLASS:	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN

SUBSTREAM: MIXED

STRUCTURE: CONVENTIONAL

H2	KMOL/HR	1155.8002	1553.6568	0.0	1553.6568	1553.6568
CO	KMOL/HR	2400.3911	2000.4127	0.0	2000.4127	2000.4127
CO2	KMOL/HR	402.7542	802.2036	0.0	802.2036	802.2036
N2	KMOL/HR	21.7460	21.7460	0.0	21.7460	1146.7461
O2	KMOL/HR	86.6950	86.6950	0.0	86.6950	86.6950
H2O	KMOL/HR	2330.0000	1931.0786	0.0	1931.0786	1931.0786
H3N	KMOL/HR	0.0	0.0	0.0	0.0	0.0
CH4	KMOL/HR	0.0	0.5319	0.0	0.5319	0.5319
H2S	KMOL/HR	61.8388	61.8388	0.0	61.8388	61.8388
TOTAL	KMOL/HR	6459.2256	6458.1636	0.0	6458.1636	7583.1636
TEMP	C	1316.0000	1316.0000	MISSING	500.0000	499.0292
PRES	ATM	58.8000	58.8000	58.8000	55.8000	47.9000
ENTHALPY	CAL/MOL	-.25384+05	-.25808+05	MISSING	-.33434+05	-.27967+05
VFRAC		1.0000	1.0000	MISSING	1.0000	1.0000
LFRAC		0.0	0.0	MISSING	0.0	0.0
ENTROPY	CAL/MOL-K	12.7977	12.6139	MISSING	6.0350	6.0668
DENSITY	MOL/CC	.44699-03	.44694-03	MISSING	.87482-03	.75058-03
AVG MW		20.8625	20.8660	MISSING	20.8660	21.9263

DESIGN OF COAL TO AMMONIA PLANT
STREAM SECTION

=====

S302 S303 S305 S308 S309

STREAM ID	S302	S303	S305	S308	S309
FROM :	M301	R302	H303	E305	E305
TO :	R302	H303	E305	K401	H306
CLASS:	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN

SUBSTREAM: MIXED

STRUCTURE: CONVENTIONAL

H2	KMOL/HR	1553.6568	3514.0612	3514.0612	3510.5472	3.5140
CO	KMOL/HR	2000.4127	40.0082	40.0082	0.2000	39.8082
CO2	KMOL/HR	802.2036	2762.6081	2762.6081	27.6260	2734.9820
N2	KMOL/HR	1146.7461	1146.7461	1146.7461	1145.5993	1.1467
O2	KMOL/HR	86.6950	86.6950	86.6950	0.4334	86.2615
H2O	KMOL/HR	2911.7786	951.3741	951.3741	0.9513	950.4227
H3N	KMOL/HR	0.0	0.0	0.0	0.0	0.0
CH4	KMOL/HR	0.5319	0.5319	0.5319	.53198-03	0.5314
H2S	KMOL/HR	61.8388	61.8388	61.8388	0.0309	61.8079
TOTAL	KMOL/HR	8563.8636	8563.8636	8563.8636	4685.3889	3878.4747
TEMP	C	466.6921	425.0000	80.0000	30.0000	30.0000
PRES	ATM	47.8000	50.0000	45.0000	45.0000	21.0000
ENTHALPY	CAL/MOL	-.31220+05	-.33620+05	-.37601+05	-548.3299	-.81086+05
VFRAC		1.0000	1.0000	0.9001	1.0000	1.0000
LFRAC		0.0	0.0	0.0998	0.0	0.0
ENTROPY	CAL/MOL-K	4.0885	1.0884	-7.0888	-6.3339	-6.6930
DENSITY	MOL/CC	.78561-03	.86602-03	0.0017	0.0017	0.0010
AVG MW		21.4784	21.4786	21.4786	8.6273	37.0036

DESIGN OF COAL TO AMMONIA PLANT
STREAM SECTION

=====

S310 S401 S401A S402 S404

STREAM ID	S310	S401	S401A	S402	S404
FROM :	H306	K401	K401A	M402	R404
TO :		K401A	M402	R404	H404A
CLASS:	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN

SUBSTREAM: MIXED

STRUCTURE: CONVENTIONAL

H2	KMOL/HR	3.5140	3510.5472	3510.5472	8273.9723	4964.3834
CO	KMOL/HR	39.8082	0.2000	0.2000	5.0010	5.0010
CO2	KMOL/HR	2734.9820	27.6260	27.6260	690.6520	690.6520
N2	KMOL/HR	1.1467	1145.5993	1145.5993	2150.7020	1047.5057
O2	KMOL/HR	86.2615	0.4334	0.4334	10.7083	10.7083
H2O	KMOL/HR	950.4227	0.9513	0.9513	23.7845	23.7845
H3N	KMOL/HR	0.0	0.0	0.0	2.1201	2208.5128
CH4	KMOL/HR	0.5314	.53198-03	.53198-03	0.0131	0.0131
H2S	KMOL/HR	61.8079	0.0309	0.0309	0.7712	0.7712
TOTAL	KMOL/HR	3878.4747	4685.3889	4685.3889	.11158+05	8951.3322
TEMP	C	-25.0000	250.0000	300.0000	300.2467	450.0000
PRES	ATM	21.0000	200.0000	300.0000	274.9000	300.0000
ENTHALPY	CAL/MOL	-.84316+05	1024.4145	1410.1865	-3954.8361	-6742.3035
VFRAC		0.7546	1.0000	1.0000	1.0000	1.0000
LFRAC		0.2453	0.0	0.0	0.0	0.0
ENTROPY	CAL/MOL-K	-15.7482	-5.5141	-5.6823	-5.1032	-7.9792
DENSITY	MOL/CC	0.0020	0.0043	0.0058	0.0053	0.0047
AVG MW		37.0036	8.6273	8.6273	9.7060	12.0985

DESIGN OF COAL TO AMMONIA PLANT
STREAM SECTION

=====

S404A S406 S407 S409 S410

STREAM ID	S404A	S406	S407	S409	S410
FROM :	H404A	D405	D405	H406	D407
TO :	D405	H406	D407		M402
CLASS:	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL				
H2	KMOL/HR	4964.3834	2.4821	4961.9012	2.4821	4763.4251
CO	KMOL/HR	5.0010	0.0	5.0010	0.0	4.8009
CO2	KMOL/HR	690.6520	0.0	690.6520	0.0	663.0259
N2	KMOL/HR	1047.5057	0.5237	1046.9820	0.5237	1005.1027
O2	KMOL/HR	10.7083	0.0053	10.7030	0.0053	10.2748
H2O	KMOL/HR	23.7845	0.0	23.7845	0.0	22.8331
H3N	KMOL/HR	2208.5128	2206.3043	2.2085	2206.3043	2.1201
CH4	KMOL/HR	0.0131	.65571-05	0.0131	.65571-05	0.0125
H2S	KMOL/HR	0.7712	0.0	0.7712	0.0	0.7403
TOTAL	KMOL/HR	8951.3322	2209.3156	6742.0166	2209.3156	6472.3360
TEMP	C	300.0000	30.0000	300.0000	-33.3000	300.0000
PRES	ATM	300.0000	3.0000	275.0000	1.5000	275.0000
ENTHALPY	CAL/MOL	-8101.4870	-.10903+05	-7838.6222	-.17019+05	-7838.6222
VFRAC		1.0000	1.0000	1.0000	0.0040	1.0000
LFRAC		0.0	0.0	0.0	0.9959	0.0
ENTROPY	CAL/MOL-K	-10.0852	-25.7512	-4.9262	-48.9017	-4.9262
DENSITY	MOL/CC	0.0060	.12361-03	0.0053	0.0105	0.0053
AVG MW		12.0985	17.0167	10.4869	17.0167	10.4869

DESIGN OF COAL TO AMMONIA PLANT
STREAM SECTION

=====

S411 S207 S301

STREAM ID	S411	S207	S301
FROM :	D407		
TO :		M204	M301
CLASS:	CONVEN	CONVEN	CONVEN

SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL		
H2	KMOL/HR	198.4760	0.0	0.0
CO	KMOL/HR	0.2000	0.0	0.0
CO2	KMOL/HR	27.6260	0.0	0.0
N2	KMOL/HR	41.8792	1125.0000	0.0
O2	KMOL/HR	0.4281	0.0	0.0
H2O	KMOL/HR	0.9513	0.0	980.7000
H3N	KMOL/HR	0.0883	0.0	0.0
CH4	KMOL/HR	.52431-03	0.0	0.0
H2S	KMOL/HR	0.0308	0.0	0.0
TOTAL	KMOL/HR	269.6806	1125.0000	980.7000
TEMP	C	300.0000	500.0000	265.0000
PRES	ATM	275.0000	48.0000	48.0000
ENTHALPY	CAL/MOL	-7838.6222	3414.7800	-.56370+05
VFRAC		1.0000	1.0000	1.0000
LFRAC		0.0	0.0	0.0
ENTROPY	CAL/MOL-K	-4.9262	-0.9230	-14.1368
DENSITY	MOL/CC	0.0053	.74374-03	0.0013
AVG MW		10.4869	28.0130	18.0150

DESIGN OF COAL TO AMMONIA PLANT
STREAM SECTION

=====

Q1

STREAM ID	Q1
FROM :	H406
TO :	
CLASS:	HEAT

STREAM ATTRIBUTES:

HEAT

Q	CAL/SEC	.37536+07
---	---------	-----------

APPENDIX C

CALCULATIONS FOR ATMOSPHERIC FLUIDIZED BED COMBUSTOR

MASS AND ENERGY BALANCES

Basis : 100 lbs of coal at a datum temperature of 77 degree F.

The amounts of various constituents present in 100 lbs of Illinois No.6 coal are presented in Table C.1. These are calculated as per the earlier Table 4.5.

The following reactions are assumed to occur during the combustion:



The following assumptions are made in this study:

1. Nitrogen present in the fuel only reacts to form NO
2. 90 percent of sulfur is captured (39)
3. Char contains 2 percent ash (39)
4. Air is pre-heated to 550 degree F

As indicated earlier, lime stone is used to capture the sulfur dioxide.

Considering a Ca/S mole ratio of 2.5, for maximum SO_2 capture,

Moles of Ca required : $2.5 \times 0.1219 = 0.3048$ lb-moles

CaO required : $0.3048 \times 56 = 17.066$ lbs = 0.305 lb moles

$CaCO_3$ required : $17.066 \times (100/56) = 30.475$ lbs

Considering 3 percent grit in the lime stone,

Lime stone required : 31.39 lbs

TABLE C.1
CONSTITUENTS IN 100 LBS OF ILLINOIS NO.6 COAL

Element	Lb-Mole
Carbon	5.525
Hydrogen	2.400
Oxygen	0.347
Sulfur	0.122
Nitrogen	0.043
Water	0.167

Theoretical oxygen required: $5.25 + 1.2 + 0.0429 + 0.01219 + 0.152$

for the above reactions = 6.657 lb moles

Nitrogen associated in air = 25.043 lb moles

Theoretical air required = 31.70 lb moles

Considering 15 percent excess air, air requirement = 36.455 lb moles

= 1057.195 lbs

Air to coal ratio (mass) = 10.57

considering a mass ratio of 11,

Air to be supplied = 1100 lbs = 37.93 lb moles

Oxygen in air = 7.965 lb moles

Nitrogen in air = 29.965 lb moles

Stack gases:

$\text{CO}_2 = 5.525 + 0.3047 = 5.83$ lb moles

$\text{H}_2\text{O} = 1.2$ lb moles

$\text{NO} = 0.086$ lb moles

$\text{O}_2 = 7.965 - 6.657 = 1.308$ lb moles

$\text{N}_2 = 29.965$ lb moles

Other materials:

Char = 10 lbs

Ash = $9.7 - 2.0 = 7.7$ lbs

Grit(SiO_2) = 0.9 lbs

Sulfur dioxide captured = $0.9 * 0.1219 = 0.10971$ lb moles

CaO utilized for SO_2 capture = $0.10971 * 56 = 6.14376$ lbs

CaO in spent lime = $17.0632 - 6.14376 = 10.9$ lbs

CaSO_4 in spent lime = $6.144 * (136/56) = 14.921$ lbs

The heat balances are performed for various items and presented in Table C.2. The heat loads for items a, b, c, i, j, k, l and m in Heat Out section are as per the literature (39). The heat capacities for air and other stack gases are from the data in the literature (40).

From the results presented in Table C.2, the heat supplied to the cold fluid in the tubes (q) is 984,402 BTU per 100 lbs of coal. From this, heat supplied for one ton of coal = 19.69 million BTU.

i) Coal requirement:

For 472 million BTU per hour of total heat load (see Table 4.4), coal supply rate will be 24 tons per hour.

Considering 80 percent combustion efficiency, the coal rate will be 30 tons per hour.

ii) Lime stone requirement:

Moles of sulfur burned = $30 \times 2000 \times 0.039 \times (1/32) = 73.125$ lb mole/hr

With Ca/S mole ratio of 2.5,

Moles of CaO required = $2.5 \times 73.125 = 182.8$ lb mole/hr = 10237.5 lb/hr

CaCO_3 required = $10237.5 \times (100/56) = 18281.25$ lb/hr = 9.14 tons/hr

Considering 3 percent grit in the lime stone,

Lime stone required = 9.42 tons/hr.

iii) Bed cross sectional area:

Mass of coal = 30 tons per hour

With a mass ratio of 11, mass of air = 330 tons/hr = 183.33 lb/sec

From the literature data (41), the density of air at 1600 degree F = 0.0197 lb/cft.

TABLE C.2

HEAT BALANCE IN AFBC

Basis:100 lbs of coal at 77 degree F

Heat In	BTU
a) Fuel consumption	1,350,000.00
b) Sensible heat of air 37.93*7.2*(550-77)	129,174.40

Total Heat In	1,479,174.40
Heat Out	
a) Calcination + Sulfation	6,265.00
b) Evaporation	4,381.90
c) Radiation(1% of heat of fuel)	13,500.00
d) Heat to cold fluid	q
Sensible heats of flue gases	
e) CO ₂ :11.1*5.83*(1600-77)	98,557.90
f) H ₂ O :1.2*9.1*(1600-77)	16,631.16
g) O ₂ :1.308*7.8*(1600-77)	15,538.26
h) SO ₂ :0.012*12*(1600-77)	219.31
i) N ₂ :29.965*7.4*(1600-77)	337,711.54
j) Char:10*52.9867	529.87
k) CaO :10.9*47.3	515.57
l) CaSO ₄ :14.92*52.058	776.71
m) Ash :7.7*18.9272	145.74

Total Heat Out	q+ 494,772.38

A superficial velocity of 8 ft/sec is considered as per the literature (59).

Then, mass of air= density of air* area of C.S * Velocity, from which

Area of bed = 1190 sq.ft

A bed of 40 ft X 30 ft is considered.

A bed depth of 6 ft is considered because the economical limit for the bed depth is about 6 ft as per the literature (51).

iv) Heat flux for catalyst tubes:

Considering an overall heat transfer coefficient of 76 BTU per hr-sq.ft.degree F as per the literature (39),

Heat transfer area required for an endothermic heat load of 232 million BTU /hr

$$=232*10^6*(1/76)*(1/(1600-1400)) = 15263.158 \text{ sq.ft}$$

Considering 4 inch O.D catalyst tubes,

Total length of tube required= 14575 ft

Considering 5 percent extra for the end connections,

Total length of tube = 15304 ft

If we further consider, 7 numbers of sub manifolds for the tubes arrangement with each sub manifold containing 60 numbers of tubes of 36 ft length,

Heat transfer area available= 15833.66 sq.ft

Heat flux =232/15833.66= 14652.33 BTU per hr-sq.ft

This is within the limits of 20,000 BTU per hr-sq.ft maximum heat

flux reported in the literature (6). The volume available for holding the catalyst is around 1100 cu.ft, which is adequate as per the literature (42). A pressure drop of 75 psi for the catalyst tubes is considered as per the literature (6). Further, if the sub manifolds are considered to be of 6 inch O.D pipes, the bed depth of 6 ft is adequate for the tube bundle with 7 numbers of sub manifolds. The tube bundle cross section will be around 37 ft X 29 ft which will fit into a bed cross section of 40 ft X 30 ft. The capacity and size of the AFBC plant in the present study are found to be within the limits of commercially available plants reported in the literature (59).

VITA

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