

**STUDIES OF THE USE OF HEAT  
FROM HIGH TEMPERATURE NUCLEAR  
SOURCES FOR HYDROGEN  
PRODUCTION PROCESSES**

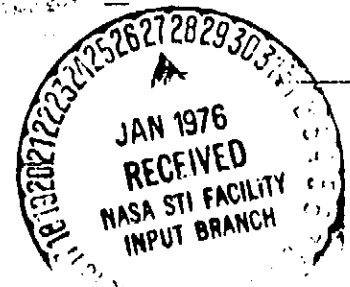
**WESTINGHOUSE ELECTRIC CORPORATION  
ASTRONUCLEAR LABORATORY**

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16. Abstract A study has been performed to assess both the future uses of hydrogen and the hydrogen production processes that can meet the demand for hydrogen in the coming decades. To do this, a projection was made of the market for hydrogen through the year 2000. Four hydrogen production processes were selected, from among water electrolysis, fossil based and thermochemical water decomposition systems, and evaluated, using a consistent set of groundrules, in terms of relative performance, economics, resource requirements, and technology status.  The market projection shows that a substantial demand for hydrogen currently exists and that the requirement grows dramatically with time. The United States currently uses about $8 \times 10^{10}$ standard cubic meters ( $3 \times 10^{12}$ SCF) of hydrogen per year. The future market indicates a year 2000 hydrogen requirement of $1.3 \times 10^{12}$ standard cubic meters ( $4.8 \times 10^{13}$ SCF) per year. This is equivalent to an average annual growth rate in excess of 11 percent.  The hydrogen production processes selected for evaluation were water electrolysis, using the Teledyne HP electrolyzer modules; coal gasification, using the Bi-Gas two stage pressurized gasifier to represent developing coal gasification technology; coal gasification, using the Koppers-Totzek atmospheric gasifier to represent commercially available coal gasification technology; and water decomposition, using the Westinghouse Sulfur Cycle hybrid thermochemical-electrochemical hydrogen production process in combination with a very high temperature nuclear reactor (VHTR) heat source. All processes were sized to produce a nominal $9.6 \times 10^6$ standard $m^3$ /day ( $360 \times 10^6$ SCFD) of hydrogen.  The evaluation indicates that the nuclear Sulfur Cycle water decomposition system is superior to water electrolysis in both thermal efficiency and cost of hydrogen produced. Nuclear water decomposition is on a par with coal gasification systems in respect to thermal efficiency and holds great promise of lower hydrogen production costs as reasonable escalation of future nuclear and coal costs are considered. The nuclear water decomposition system has a lower potential environmental impact than other systems. It also provides the opportunity for more effective resource management, such as making possible the utilization of all the carbon in coal for its chemical value, as opposed to converting it to carbon dioxide while extracting only its thermal value.					
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## TABLE OF CONTENTS

		<u>Page</u>
	SUMMARY	xi
1.0	INTRODUCTION	1- 1
2.0	HYDROGEN MARKET PROJECTION	2- 1
2.1	GENERAL	2- 1
2.2	PREDICTED TOTAL HYDROGEN MARKET	2- 1
2.3	MARKET FOR HYDROGEN IN FUEL SYNTHESIS	2- 3
	2.3.1 Hydrogen Market in Gaseous Fuel Synthesis	2- 3
	2.3.2 Hydrogen Market in Liquid Fuel Synthesis	2- 6
	2.3.3 Hydrogen Market in the Projection of Other Synthetic Fuels	2- 6
	2.3.4 Nuclear Hydrogen Market in Fuel Synthesis	2- 6
2.4	HYDROGEN MARKET IN STEELMAKING	2- 8
	2.4.1 Market for Hydrogen in Direct Reduction Steelmaking	2-11
	2.4.2 Market for Nuclear Hydrogen in Direct Reduction Steelmaking	2-11
2.5	MARKET FOR HYDROGEN IN THE PRODUCTION OF AMMONIA	2-14
	2.5.1 Present Trends in the United States Ammonia Market	2-14
	2.5.2 The World Ammonia Market	2-14
	2.5.3 Total Hydrogen Market in Ammonia Production	2-16
	2.5.4 Market for Nuclear Hydrogen in Ammonia Production	2-16
2.6	MARKET FOR HYDROGEN AS A FUEL	2-16
	2.6.1 Market for Nuclear Hydrogen as a Fuel	2-20
	2.6.2 Market for Solar Hydrogen as a Fuel	2-20
2.7	MARKET FOR HYDROGEN IN OIL REFINING	2-23
	2.7.1 Projected Total Hydrogen Use in Oil Refining	2-23
	2.7.2 Nuclear Hydrogen Use in Oil Refining	2-25
2.8	AREAS OF UNCERTAINTY	2-25
3.0	SELECTION OF HYDROGEN PRODUCTION SYSTEMS FOR EVALUATION	3- 1
3.1	GENERAL	3- 1

## TABLE OF CONTENTS (Continued)

		<u>Page</u>
3.2	WATER ELECTROLYSIS HYDROGEN PRODUCTION SYSTEMS	3- 3
3.2.1	State-of-the-Art	3- 3
3.2.2	Theoretical Background	3- 3
3.2.3	Comparative Data on Electrolyzers	3- 7
3.2.4	Environmental Constraints	3-14
3.2.5	Water Electrolysis Plants	3-15
3.2.6	Electrolyzer Selection	3-15
3.3	FOSSIL BASED HYDROGEN PRODUCTION PROCESSES	3-17
3.3.1	General	3-17
3.3.2	Selection of Type of Fossil Based Hydrogen Production System to be Studied	3-17
3.3.3	Coal Gasification Systems	3-20
3.4	WATER DECOMPOSITION HYDROGEN PRODUCTION SYSTEMS	3-29
3.4.1	Water Splitting Processes as a Class of Hydrogen Generation Methods	3-30
3.4.2	Basis of Selecting a Water Decomposition System	3-37
3.4.3	Westinghouse Water Decomposition Process	3-60
3.4.4	Energy Sources for the Westinghouse Sulfur Cycle	3-65
4.0	TECHNICAL AND ECONOMIC EVALUATION OF SELECTED HYDROGEN PRODUCTION PROCESSES	4- 1
4.1	GENERAL	4- 1
4.1.1	Technical Groundrules for Evaluation	4- 1
4.1.2	Economic Groundrules for Evaluation	4- 3
4.2	WATER ELECTROLYSIS	4- 6
4.2.1	General	4- 6
4.2.2	Plant Design	4- 8
	4.2.2.1 Electrolyzers	4- 8
	4.2.2.2 Plant Subsystems	4-10
	4.2.2.3 Water Make-Up System	4-14
	4.2.2.4 Electrolyte Preparation and Storage System	4-14
	4.2.2.5 Heat Removal System	4-14
	4.2.2.6 Product Gas Handling	4-16
	4.2.2.7 Electrical Auxilairy Power System	4-16
	4.2.2.8 Plant Maintenance	4-16

## TABLE OF CONTENTS (Continued)

		<u>Page</u>
4.2.3	Plant Performance Characteristics	4-16
	4.2.3.1 Resource Consumption	4-16
	4.2.3.2 Process Outflows	4-19
	4.2.3.3 Process Thermal Efficiency	4-19
4.2.4	Economics	4-22
	4.2.4.1 Capital Costs	4-22
	4.2.4.2 Operation and Maintenance Costs	4-26
	4.2.4.3 Power Costs	4-26
	4.2.4.4 Hydrogen Production Costs	4-30
	4.2.4.5 Sensitivity of Hydrogen Production Costs to Variables	4-30
4.3	Bi-GAS COAL GASIFICATION	4-37
4.3.1	General	4-37
4.3.2	The Bi-Gas Process	4-37
4.3.3	Hydrogen Production Plant	4-42
4.3.4	Plant Performance Characteristics	4-46
	4.3.4.1 Resource Consumption	4-46
	4.3.4.2 Process Outflows	4-48
	4.3.4.3 Process Thermal Efficiency	4-48
4.3.5	Economics	4-49
	4.3.5.1 Capital Costs	4-49
	4.3.5.2 Operation and Maintenance Costs	4-53
	4.3.5.3 Fuel Costs	4-57
	4.3.5.4 Hydrogen Production Costs	4-57
	4.3.5.5 Sensitivity of Hydrogen Production Costs to Variables	4-57
4.3.6	Alternate Configuration - Dual Purpose Bi-Gas Process	4-59
4.4	KOPPERS-TOTZEK COAL GASIFICATION	4-65
4.4.1	General	4-65
4.4.2	The Koppers-Totzek Process	4-65
4.4.3	Hydrogen Production Plant	4-72
	4.4.3.1 General	4-72
	4.4.3.2 Coal Preparation	4-72
	4.4.3.3 Gasification	4-76
	4.4.3.4 Acid Gas Removal	4-76
	4.4.3.5 CO Shift Conversion	4-76
	4.4.3.6 CO <sub>2</sub> Removal	4-80

## TABLE OF CONTENTS (Continued)

	<u>Page</u>
4.4.3.7 Polishing Methanation.....	4-80
4.4.3.8 Plant Service Systems	4-80
4.4.3.8.1 Oxygen Plant	4-80
4.4.3.8.2 Cooling Water	4-33
4.4.3.8.3 Water Make-Up	4-83
4.4.3.8.4 Steam Generation	4-83
4.4.3.8.5 Waste Disposal	4-83
4.4.3.8.6 Electrical Distribution	4-84
4.4.4 Plant Performance Characteristics	4-84
4.4.4.1 Resource Consumption	4-84
4.4.4.2 Process Outflows	4-84
4.4.4.3 Process Thermal Efficiency	4-84
4.4.5 Economics	4-87
4.4.5.1 Capital Costs	4-87
4.4.5.2 Operation and Maintenance Costs	4-90
4.4.5.3 Fuel Costs	4-93
4.4.5.4 Hydrogen Production Costs	4-93
4.4.5.5 Sensitivity of Hydrogen Production Costs to Variables	4-96
4.5 WATER DECOMPOSITION	4-99
4.5.1 General	4-99
4.5.2 Plant Design	4-99
4.5.2.1 Plant Layout	4-99
4.5.2.2 The Very High Temperature Reactor (VHTR)	4-103
4.5.2.3 Battery G - Electrolyzer	4-110
4.5.2.4 Battery H - Sulfuric Acid Decomposition	4-111
4.5.2.5 Battery I - SO <sub>2</sub> /O <sub>2</sub> Separation	4-113
4.5.2.6 Battery J - Turbine Generator	4-113
4.5.2.7 Battery K - Hydrogen Product Compressors	4-117
4.5.2.8 Cooling Water System	4-117
4.5.2.9 Water Make-Up and Waste Treatment Systems	4-117
4.5.2.10 Electrical Auxiliary Power System	4-118
4.5.2.11 General Facilities	4-119

## TABLE OF CONTENTS (Continued)

		<u>Page</u>
4.5.3	Plant Reference Characteristics	4-119
4.5.3.1	Resource Consumption	4-119
4.5.3.2	Process Outflows	4-120
4.5.3.3	Process Thermal Efficiency	4-120
4.5.4	Process Performance Sensitivity Analysis	4-121
4.5.5	Economics	4-136
4.5.5.1	Capital Costs	4-136
4.5.5.2	Operation and Maintenance Costs	4-142
4.5.5.3	Fuel Costs	4-144
4.5.5.4	Hydrogen Production Costs	4-144
4.5.5.5	Sensitivity of Hydrogen Production Costs to Variables	4-147
5.0	COMPARATIVE EVALUATION OF HYDROGEN PRODUCTION PROCESSES	5- 1
5.1	GENERAL	5- 1
5.2	COMPARISON OF TECHNOLOGICAL READINESS AND DEVELOPMENT REQUIREMENTS	5- 1
5.2.1	Water Electrolysis	5- 1
5.2.2	Koppers-Totzek Coal Gasification	5- 2
5.2.3	Bi-Gas Coal Gasification	5- 3
5.2.4	Water Decomposition System	5- 4
5.2.4.1	The VHTR Nuclear Heat Source	5- 4
5.2.4.2	The Water Decomposition System	5- 5
	5.2.4.2.1 Materials Considerations	5- 5
	5.2.4.2.2 Technological Status of the Water Decomposition Hydrogen Generation Process	5- 5
5.3	ECONOMIC COMPARISON OF HYDROGEN PRODUCTION PROCESSES	5- 6
5.3.1	Capital Costs	5- 6
5.3.2	Comparison of Operating and Maintenance Costs	5- 8
5.3.3	Comparison of Fuel Costs	5- 8
5.3.4	Comparison of Hydrogen Production Costs	5-12



TABLE OF CONTENTS (Continued)

	<u>Page</u>	
5.4	COMPARISON OF RESOURCE UTILIZATION AND ENVIRONMENTAL IMPACT POTENTIAL	5-16
6.0	SUMMARY OF RESULTS	6- 1
6.1	HYDROGEN MARKET PROJECTION	6- 1
6.2	HYDROGEN PRODUCTION PROCESSES	6- 2
	6.2.1 Water Electrolysis	6- 2
	6.2.2 Bi-Gas Coal Gasification	6- 4
	6.2.3 Koppers-Totzek Coal Gasification	6- 4
	6.2.4 Nuclear Water Decomposition	6- 4
6.3	CONCLUSIONS	6- 6
	APPENDIXES	
A	Materials for the Sulfur Cycle Water Composition System	A-1 - A-11
B	Technology Status of the Sulfur Cycle Water Decomposition System	B-1 - B-22
	REFERENCES	1 - 4

## SUMMARY

A study has been performed to assess both the future uses of hydrogen and the hydrogen production processes that can meet the demand for hydrogen in the coming decades. To do this, a projection was made of the market for hydrogen, as a fuel and as a feedstock, through the year 2000. Four hydrogen production processes were selected, from among water electrolysis, fossil based and thermochemical water decomposition systems, and evaluated, using a consistent set of groundrules, in terms of relative performance, economics, resource requirements, and technology status.

### Market Projection

The market projection shows that a substantial demand for hydrogen currently exists and that the requirement grows dramatically with time. The United States currently uses about  $8 \times 10^{10}$  standard cubic meters ( $3 \times 10^{12}$  SCF) of hydrogen per year, with a growth rate that is approximately six percent per year. As one looks to the future, and the growing markets for merchant hydrogen that do not now exist, e.g., coal gasification and liquefaction, ore reduction, fuel, etc., the projection for the year 2000 hydrogen market becomes  $1.3 \times 10^{12}$  standard cubic meters ( $4.8 \times 10^{13}$  SCF) per year. This is equivalent to an average annual growth rate in excess of 11 percent compared to the historical six percent rate.

### Hydrogen Production Processes

The hydrogen production processes selected for evaluation were water electrolysis, using the Teledyne HP electrolyzer modules; coal gasification, using the Bi-Gas two stage pressurized gasifier to represent developing coal gasification technology; coal gasification, using the Koppers-Totzek atmospheric gasifier to represent commercially available coal gasification technology; and water decomposition, using the Westinghouse Sulfur Cycle thermochemical hydrogen production process in combination with a very high temperature nuclear reactor (VHTR) heat source.

The technology of water electrolysis is well known and electrolyzers are available commercially from many manufacturers. The thermal efficiency of the water electrolysis plant is 81 percent, not including the efficiency of producing the electric power required for the process. When the electric generation efficiency is included at 34 percent, typical of the light water nuclear reactor powerplants capable of producing the lowest cost electric power currently available, the combined overall process efficiency drops to about 28 percent. The cost of producing hydrogen from this plant, based on utility ownership and costs in effect in mid-1974, is estimated to be approximately 8.47¢/std m<sup>3</sup> (\$2.27/MSCF) when operating at an 80 percent capacity factor and supplied with power from an adjacent nuclear power station with a fuel cost of 19.9¢/GJ (21¢/10<sup>6</sup> Btu).

The Bi-Gas gasifier is a two stage pressurized system which represents developing technology in coal gasification. The overall thermal efficiency of the plant, relating the higher heating value of the product gas to the total energy input to the plant, was calculated

to be 46 percent. The cost of the production facility included, as in all the processes, equipment and facilities, such as cooling towers and flue gas cleanup systems, to assure that the plants would meet the appropriate environmental standards and regulations. The cost of producing hydrogen from this plant, under base case economic conditions, is 4.46¢/std m<sup>3</sup> (\$1.20 MSCF). The base case considered coal at 2.2¢/kg (\$20/ton).

Koppers-Totzek gasification is a commercially available process. Gasification plants using these gasifiers are in existence around the world. The gasifier, which operates at approximately atmospheric pressure, can handle any kind of coal and, with appropriate downstream processing, produce a hydrogen product stream. Compression stages were included in the plant to result in the product gas being available at a pressure of 6895 kPa (1000 psi), as for the other hydrogen production systems, for off-site distribution. The overall thermal efficiency of the process, including the energy consumed in gas compression and other plant services, is evaluated to be 49 percent. The base economic evaluation resulted in a hydrogen production cost of 5¢/std m<sup>3</sup> (\$1.34/MSCF).

The water decomposition system used for evaluation is the Westinghouse Sulfur Cycle two-step thermochemical process. In this process, hydrogen and sulfuric acid are produced electrolytically by the reaction of sulfur dioxide and water. The process is completed by vaporizing the sulfuric acid and thermally reducing, at higher temperatures, the resultant sulfur trioxide into sulfur dioxide and oxygen. Following separation, sulfur dioxide is recycled to the electrolyzer and oxygen is either vented or sold.

As in conventional water electrolysis, hydrogen is produced at the electrolyzer cathode. Unlike water electrolysis, sulfuric acid, rather than oxygen, is produced at the anode. Operation in this fashion reduces the theoretical power required per unit of hydrogen production by more than 85 percent over that required in water electrolysis. This is partially offset, however, by the need to add thermal energy to the process to reduce the sulfur trioxide. Even so, this hydrogen generation process provides overall thermal efficiencies approximately double those attainable by conventional electrolytic hydrogen and oxygen production technology. The development effort on the water decomposition system has, to date, been privately funded and has verified, by laboratory testing, that the electrolytic and chemical reactions proceed as written and at rates sufficient to insure an efficient and economic hydrogen production plant.

The energy source for the water decomposition system is a very high temperature nuclear reactor (VHTR) producing both electric power and a high temperature helium stream to the process. The VHTR is a graphite moderated helium cooled nuclear unit that is predicated on the integration of the technologies from the NERVA nuclear rocket engine program and land based gas cooled reactor programs into an advanced very high temperature nuclear heat and power source. The conceptual design of the VHTR was sponsored by ERDA and is described in Reference 1.

The integrated plant requires a VHTR rated at 3220 MW(t) to result in the production of  $10.1 \times 10^6$  std  $m^3$ /day ( $379 \times 10^6$  SCFD) of 99.9 percent pure hydrogen. The VHTR provides all of the energy - heat and electricity - required for the operation of the water decomposition plant and for the auxiliary power requirements of the nuclear system. The overall thermal efficiency of the integrated process is calculated to be 47 percent. For the base economic case, nuclear fuel costs of 24.75¢/GJ (26.1¢/10<sup>6</sup> Btu), and no credit for the oxygen produced in the process, the hydrogen production cost is 5.4¢/std  $m^3$  (\$1.45/MSCF).

### Conclusions

There is a market for hydrogen that exists today that is being met primarily by fossil based hydrogen production processes. This market is expected to grow substantially over the next several decades. Simultaneously, the growing unavailability and/or escalating costs of the fossil feedstocks used in today's hydrogen production makes imperative the development of alternative hydrogen generation systems. These systems must make use of our most plentiful resources, i.e., they must be nuclear or coal based systems.

The evaluation of the nuclear Sulfur Cycle water decomposition system indicates that it is superior to water electrolysis in both thermal efficiency and cost of hydrogen produced, regardless of whether the water electrolysis plant is powered by nuclear-electric or fossil-electric plants. Nuclear water decomposition is on a par with coal gasification systems in respect to thermal efficiency and holds great promise of lower hydrogen production costs as reasonable escalation of future nuclear and coal costs are considered. The nuclear water decomposition system has a lower potential environmental impact than other systems. It also provides the opportunity for more effective resource management, such as making possible the utilization of all the carbon in coal for its chemical value, as opposed to converting it to carbon dioxide while extracting only its thermal value.

It is concluded that the nuclear water decomposition system shows sufficient technological and economic promise to warrant aggressive development of the process and further definition of the conceptual design.

## 1.0 INTRODUCTION

The objectives of the "Studies of the Use of Heat from High Temperature Nuclear Sources for Hydrogen Production Processes" are:

- To survey existing and advanced processes for the production of hydrogen by use of fossil, nuclear, and other energy sources or appropriate combinations thereof.
- To analyze and evaluate these various processes in terms of cost, energy supply, environmental impact, critical materials, and other factors; to assess the status of technology for the promising processes; and to specify the R&D needed to make the promising processes practical.
- To prepare a conceptual design of a hydrogen-production plant based on one of the most promising processes; and for this process, to prepare program plans for the needed R&D and demonstration at the pilot-plant scale.

To achieve these objectives, a scope of effort has been undertaken which is divided into three major technical tasks. These tasks are summarized below:

- TASK I - Identification of Candidate Processes for Production and Market Surveys for Uses of Hydrogen

The results of this task will be a comparative evaluation of various hydrogen generation processes supporting the selection of the electrolysis, coal gasification, and water decomposition processes to be studied in more detail; preliminary technical, environmental, and sociological information pertinent to the selected hydrogen generation processes; and projections, to the year 2000, of the market demand for hydrogen as a fuel, feedstock, or reagent.

- TASK II - Technical Analyses and Economic Evaluation of Hydrogen Production Systems

This task will result in a more detailed evaluation of the four hydrogen production processes selected in Task I, i.e., electrolysis using the Teledyne HP modules, coal gasification using the Koppers-Totzek atmospheric gasifier, coal gasification using the Bi-Gas pressurized gasifier, and thermochemical using the Westinghouse Sulfur Cycle. The evaluation will consider the economics, technical status, R&D requirements, resource requirements, environmental impacts, and other factors that bear on a recommendation of a hydrogen production process that can best meet the requirements of the market identified in Task I.

- **TASK III - Conceptual Design of a Plant for Hydrogen Production**

The results of this task will be a conceptual design of an integrated nuclear-hydrogen production plant, using the Westinghouse Sulfur Cycle hydrogen production process, including an evaluation of the economics, environmental effects, benefits, and the program, in respect to technical areas, costs, and schedules, needed to develop the hydrogen production system to the demonstration stage.

This report documents the results of Tasks I and II. The results of Task III are reported in a separate document.

In performing this work, it was recognized that ERDA-Nuclear Energy is conducting studies to assess the potential for development of nuclear systems to provide process heat at temperatures in the range of 922 to 1366K (1200 to 2000°F). These ERDA studies are also concerned with identifying and evaluating present and projected industrial processes that can utilize high temperature nuclear heat. NASA is participating in the ERDA evaluation through the assessment of processes for hydrogen production using nuclear, as well as fossil, heat sources as reported herein.

In order to make the results of this work most useful to ERDA, the hydrogen production capacity of the systems investigated was established consistent with the size of nuclear heat sources being considered in the ERDA evaluation. This results in a nominal hydrogen generation rate of  $9.6 \times 10^6$  standard cubic meters per day ( $360 \times 10^6$  SCFD) (1). Moreover, the methodology and format for estimating capital, operating, and production costs are consistent with those used by ERDA-Nuclear Energy in their studies of the very high temperature nuclear heat sources.

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(1) Throughout this report, the standard cubic meter is defined as a gas volume at normal atmospheric pressure and a temperature of 273K (32°F). The standard cubic foot is defined as a gas volume at normal atmospheric pressure and a temperature of 289K (60°F).

## 2.0 HYDROGEN MARKET PROJECTION

### 2.1 GENERAL

In this study, both the total market for hydrogen as a fuel or feedstock and the sector of the market that could be filled by nuclear driven hydrogen production systems were examined. The nuclear sector is of primary concern because it introduces new options, e.g., the shift to a nuclear energy base with its accompanying economic and environmental advantages. The basic projection is related to the growth of the hydrogen market through the year 2000, although indications of the expected growth beyond that point are also shown.

In many respects, the current production of hydrogen is not really a true market for hydrogen per se, since most of the processes involved, e.g., ammonia production, do not purchase hydrogen externally but are designed around a hydrocarbon reforming process. Although hydrogen-consuming processes could be supplied from an external hydrogen process, in today's climate this approach would appear to be less economical and less thermally efficient than existing processes which integrate both functions.

### 2.2 PREDICTED TOTAL HYDROGEN MARKET

The United States currently uses about  $80 \times 10^9$  std m<sup>3</sup> (3 TCF\*) of hydrogen per year. Production is growing today at 6 percent a year, and is expected to grow even more rapidly. This study predicts about  $1298 \times 10^9$  std m<sup>3</sup>/year (48 TCF/year) as a base case for the year 2000. Equally plausible predictions by others range to  $1660 \times 10^9$  std m<sup>3</sup>/year (62 TCF/year). Continued expansion at the present rate of 6 percent/year would result in  $402 \times 10^9$  std m<sup>3</sup>/year (15 TCF/year) by the year 2000. Table 2.2.1 summarizes some of these estimates, based on interpretations of published work. Noteworthy are the differences between forecasts as to the size and composition of the A.D. 2000 market.

The largest potential market in view is the synthetic hydrocarbon fuel market, consisting of the production of substitute natural gas (SNG) and oil from coal. Similarly, large markets in oil refining and ammonia production can be anticipated, but the magnitude of these markets is uncertain. Direct-reduction steelmaking is not seen to be a relatively large market, primarily because of the slow growth projected for the United States steel industry.

Hydrogen for fuel uses will be a relatively small market, at least through 2000 A.D., but one that will grow rapidly thereafter. However, hydrogen will not be a "universal fuel" even in the nuclear era commencing in the next century, although it is destined to be increasingly important. The basis for this judgment is predicated on the assumption that hydrogen will not be made from coal for use as a fuel because the advantages of SNG, in production cost and

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\* TCF, or Trillion Cubic Feet, is defined as  $1 \times 10^{12}$  standard cubic feet

TABLE 2.2.1

PROJECTED YEAR 2000 HYDROGEN CONSUMPTION IN THE UNITED STATES

UNITS:  $10^9$  Std  $m^3$ /Year

	Total $H_2$	Coal-SNG Coal Syncline Shale Oil	Ammonia and Chemical	Steelmaking and Metals	Direct Use As Fuel	Oil Refining
<u>This Work</u>	638 1298 1704	512 907 1172	67 129 188	8 16 32	0 34 100	51 212 212
<u>Bureau of Mines</u> 1970 Mineral Facts and Problems (1)	161 242 1663	0 0 1233	67 83 120	2 2 16	0 0 0	61 124 212
Adkins 75 (2) (Tentative)	242 322 724	88 153 509	75 94 116	10 14 19	0 0 0*	59 61 73
<u>Hydrocarbon Processing 3/74 (3)</u>	348 885	52 589	150 150	37 37	0 0	102 102
<u>Russell 74 (4)</u>	335 1392	- 1394	147 147	0 0	0 0	187 187
<u>Hoffman 74 (5)</u>	579	347	347	347	316	347

\* As a contingency the Bureau of Mines suggests  $14 \times 10^9$  std  $m^3$ /year fuel use.

- 1. Reference 2
- 2. Reference 3
- 3. Reference 4
- 4. Reference 5
- 5. Reference 6



pipeline transport cost, outweigh any identified advantage of hydrogen in end use, either in economic terms or in the conservation of coal resources.

Table 2.2.2 shows the nuclear hydrogen production capacity predicted to exist by the year 2000 A.D. The central value of  $104.3 \times 10^9$  std  $m^3$ /year (3.6 TCF/year) represents a fairly likely combination of the first commercial use, in 1995, of the very high temperature nuclear heat source (VHTR) and a water decomposition system, coupled with a moderate rate of capture of the new plant market. The rapidly growing fuel synthesis market is expected to be the dominant application of nuclear hydrogen, followed by hydrogen production for aircraft fuel and possibly dilution of methane in natural gas distribution systems. The base estimate of nuclear driven hydrogen production processes would require 15-30 3000 MW(t) VHTR's by 2000 A.D.

### 2.3 MARKET FOR HYDROGEN IN FUEL SYNTHESIS

Almost all fuel hydrocarbon processing involves the transformation of low hydrogen content materials, e.g., crude oil at 11 - 14 percent hydrogen or coal at 5 percent hydrogen, by weight, to more volatile, more useable and more valuable materials such as gasoline ( $C_8H_{18}$ ), at 16 percent hydrogen, and methane ( $CH_4$ ), at 25 percent hydrogen. Closely related processes generate methanol ( $CH_3OH$ ) and ammonia ( $NH_3$ ), also useable as fuels because of their hydrogen content and consequent high heat of combustion.

The amount of hydrogen used in the production of fuels is highest for methane (SNG) and lowest for shale oil production and oil refining. In this section, three markets are considered: coal gasification, coal liquefaction, and shale oil production. All three are substitute fuels, but the extent to which hydrocarbons are transformed and the amount of hydrogen required are greater for the two coal conversion processes. Table 2.3.1 summarizes the projected United States hydrogen demand for fuel synthesis in the year 2000.

#### 2.3.1 Hydrogen Market in Gaseous Fuel Synthesis

The volume of future synthetic gaseous fuel production in the United States is uncertain in the long term. Estimates from the literature have indicated that year 2000 production of substitute natural gas (SNG) ranges from  $80$  to  $160 \times 10^9$  std  $m^3$ /year (3 to 6 TCF/year), (Reference 7).

It was assumed for both base and high estimates that the year 2000 annual production of SNG from both coal and oil is  $169 \times 10^9$  std  $m^3$  (6.3 TCF) increasing to  $482 \times 10^9$  std  $m^3$  (18 TCF) of SNG in the year 2020. This estimate is consistent with the Project Independence "Accelerated" scenario projection (Reference 7). Assuming 1.56 standard volumes of hydrogen required per standard volume of SNG, the associated hydrogen demand is  $265 \times 10^9$  std  $m^3$ /year (9.9 TCF/year) in 2000 and  $752 \times 10^9$  std  $m^3$ /year (28 TCF/year) in 2020. For a low estimate,  $161 \times 10^9$  std  $m^3$  (6 TCF) of hydrogen was used.

TABLE 2.2.2

NUCLEAR HYDROGEN INSTALLED CAPACITY, 2000 A.D.  
UNDER VARIOUS ASSUMPTIONS

		Nuclear Process Commercial Availability		
		Late	Intermediate	Early
		2000	1995	1990
		$10^9$ Std $m^3$ /Yr	$10^9$ Std $m^3$ /Yr	$10^9$ Std $m^3$ /Yr
<u>Slow Capture Rates</u>				
Oil Refining	5%/Yr	0	4.6	19.9
Fuel Synthesis	↓	↓	27.3	118
Chemical	↓	↓	3.0	12.3
Steelmaking	↓	↓	0.7	3.1
Direct Fuel	1%/Yr	↓	<u>17.2</u>	<u>74.3</u>
Total		0	52.8	227.6
<u>Moderate Capture Rates</u>				
Oil Refining	10%/Yr	0	9.2	39.8
Fuel Synthesis	↓	↓	54.4	235.8
Chemical	↓	↓	5.7	24.7
Steelmaking	↓	↓	1.4	6.2
Direct Fuel	2%/Yr	↓	<u>33.6</u>	<u>148</u>
Total		0	104.3	454.5
			(Base Estimate)	
<u>Fast Capture Rates</u>				
Oil Refining	20%/Yr	0	18.5	61.1
Fuel Synthesis	↓	↓	108.8	371.9
Chemical	↓	↓	11.6	37.7
Steelmaking	↓	↓	2.9	9.6
Direct Fuel	5%/Yr	↓	<u>84.4</u>	<u>367</u>
Total		0	226.2	847.3
			(High Estimate)	

TABLE 2.3.1

## UNITED STATES HYDROGEN DEMAND FOR FUEL SYNTHESIS, 2000 A.D.

Product	Product Demand	Hydrogen Energy Product Energy	Hydrogen Demand	
	$10^{18}$ J/Year		$10^{18}$ J/Year	$10^9$ Std m <sup>3</sup> /Year
<u>Low Estimate</u>				
SNG	4.2	0.491	2.06	161
Synchrude	9.5	0.392	3.72	291
Shale Oil	10.5	0.073	<u>0.77</u>	<u>60</u>
Total	24.2		6.55	512
<u>Best Estimate</u>				
SNG	6.9	0.491	3.39	265
Synchrude	19.0	0.392	7.45	582
Shale Oil	10.5	0.073	<u>0.77</u>	<u>60</u>
Total	36.4		11.61	907
<u>High Estimate</u>				
SNG	6.9	0.491	3.39	265
Synchrude	29.5	0.392	11.6	907
Shale Oil <sup>(1)</sup>	-	-	<u>-</u>	<u>-</u>
Total	36.4		14.99	1172

(1)

For the high estimate, shale oil is assumed no-viable and its energy contribution is replaced by additional Synchrude.

### 2.3.2 Hydrogen Market in Liquid Fuel Synthesis

The base year 2000 market for synthetic liquid fuels from coal was assumed to be about 3.1 billion barrels of oil, and that production of oil from shale amounts to an additional 1.7 billion barrels oil. These numbers approximate the upper limit estimates published by the Bureau of Mines in 1970 (Reference 2). The associated total annual hydrogen demands are 188 std m<sup>3</sup>/barrel (7000 SCF/barrel) and 35 std m<sup>3</sup>/barrel (1300 SCF/barrel), yielding 582 × 10<sup>9</sup> std m<sup>3</sup> (21.7 TCF) and 60 × 10<sup>9</sup> std m<sup>3</sup> (2.2 TCF), respectively. The unit hydrogen demand in oil shale production is much less than in fuel synthesis from coal; thus the total hydrogen market would be less if shale oil is very successful. On the other hand, if shale oil fails to become viable in this century (e.g., due to its waste product volume) and the United States elects to limit oil imports, the hydrogen demand would increase to 907 × 10<sup>9</sup> std m<sup>3</sup> (34 TCF), given the same total energy demand of 4.8 billion barrels of synthetic oil. The value was used as a high estimate. The hydrogen requirement of the syncrude industry is the largest part of the fuels market and in fact constitutes over 60 percent of the base case projection. The total A.D. 2000 base fuel synthesis industry assumed here amounts to 36.4 × 10<sup>18</sup> J/year. Project Independence investigators utilized a base demand of 33.7 × 10<sup>18</sup> J(32 quads\*) (Reference 7).

### 2.3.3 Hydrogen Market in the Projection of Other Synthetic Fuels

While it seems unlikely that ammonia will replace methane, methanol produced from coal is not unlikely as a liquid synthetic fuel candidate. The efficiency of conversion of coal to methanol is poorer than for SNG production, since methanol production from coal involves first producing hydrogen and then combining it with carbon monoxide.

If methanol replaced gasoline as the basis of transportation energy, the hydrogen requirement would be tripled. This study did not consider the scenario in which a high consumption level of liquid fuels is met with methanol from coal. The hydrogen estimates made previously are intended to include all synthetic hydrocarbon fuels.

### 2.3.4 Nuclear Hydrogen Market in Fuel Synthesis

The rate at which nuclear-modified processes can enter this market depends upon the new hydrogen capacity added each year. It was assumed that plants will not be retrofitted and existing plants would not be retired. Since the nuclear system is assumed to be available in 1990 or later, only the new plant additions after 1990 are accessible to a nuclear-driven process. Table 2.3.2 develops an estimate of this nuclear hydrogen penetration of the SNG market. The table shows the growth in installed SNG production capacity and new capacity additions in successive five-year intervals through the year 2030. Also shown are the cumulative nuclear process additions computed for a nuclear process entering the market in 1990 or 1995 and thereafter capturing 5, 10, and 20 percent per year

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1 quad = quadrillion Btu = 10<sup>15</sup> Btu

TABLE 2.3.2  
ESTIMATED TOTAL SNG CAPACITY AND SNG CAPACITY  
BASED ON NUCLEAR-HYDROGEN

Year	Projected SNG Market ( $10^{18}$ J of SNG/Year)		Cumulative Installed Nuclear SNG Capacity ( $10^{18}$ J of SNG/Year)					
	Installed SNG Capacity at Start	Capacity Additions In 5 Years	Market Penetration Rate for 1990 Entry			Market Penetration Rate for 1995 Entry		
			5%/Yr	10%/Yr	20%/Yr	5%/Yr	10%/Yr	20%/Yr
1985	1.48		0	0	0	0	0	0
1990	3.06	1.58	0	0	0	0	0	0
1995	4.74	1.68	0.17	0.34	0.67	0	0	0
2000	6.85	2.11	0.91	1.81	2.78	0.21	0.42	0.84
2005	9.07	2.22	2.24	4.03	5.00	0.99	1.98	3.06
2010	11.8	2.73	4.56	6.76	7.73	2.63	4.71	5.79
2015	15.3	3.50	8.06	10.3	11.2	5.60	8.21	9.29
2020	19.5	4.20	12.8	14.5	15.4	9.80	12.4	13.5
2025	23.8	4.30	17.1	18.8	19.7	14.1	16.7	17.8
2030	28.2	4.40	21.5	23.2	24.1	18.5	21.1	22.2

of new plant additions. For the 5 percent/year trend, the nuclear hydrogen process is assumed to capture none of the market in the first year, 5 percent of the new plant additions the second, and so on.

If the calculation were done on a yearly basis, one would simply multiply the new plant additions in the years 1990, 1991, 1992, . . . by the fractions 0, 0.05, 0.10, . . . to obtain the annual additions and then sum these to find the installed nuclear capacity. Since this would require a lengthy table, five-year intervals were used instead. The series of annual market captures for the 5 percent/year trend was converted to average captures over successive five-year intervals, giving 0.10, 0.35, 0.60, 0.85, 1.0, 1.0, . . . . . The five year average captures for the 10 percent/year trend are 0.20, 0.70, 1.0, 1.0, . . . , and for the 20 percent/year trend are 0.4, 1.0, 1.0, . . . . .

Taking 1990 VHTR availability and the slowest rate of market penetration as an example, the nuclear process captures 10 percent of the  $1.68 \times 10^{18}$  J of new SNG capacity built between 1990 and 1995. In the next five year interval, 35 percent of the  $2.11 \times 10^{18}$  J of new plant capacity, or  $0.74 \times 10^{18}$  J additional nuclear capacity are built, bringing the total nuclear capacity in 2000 to  $0.91 \times 10^{18}$  J. This amounts to 13 percent of the year 2000 SNG production capacity of  $6.85 \times 10^{18}$  J.

In Table 2.3.3 a projected coal liquefaction industry reaching  $19.0 \times 10^{18}$  J per year of synthetic liquid fuel by 2000 A.D. is used as a basis. The same curve of market growth has been assumed as for the gasification industry. As a result, the installed process capacity for a given nuclear process entry date and capture rate is the same as before. For example, the 1990/5 percent per year combination achieves  $2.51 \times 10^{18}$  J/year capacity by 2000, or 13 percent of the total liquefaction industry.

Table 2.3.4 summarizes the coal gasification and liquefaction market volumes in terms of annual hydrogen production capacity in the year 2000. The portion of that market that can be satisfied by nuclear driven hydrogen production processes, as a function of time of entry into the market and rate of market penetration, is also shown.

## 2.4 HYDROGEN MARKET IN STEELMAKING

In contrast to other markets, the use of hydrogen in steelmaking depends upon the reducing property of hydrogen rather than its propensity to bond with carbon. Very little hydrogen is used in this way today --- the United States produces about one million tons of steel annually by the direct reduction process, using hydrogen obtained by cracking methane. At about  $820 \text{ std m}^3/\text{kg}$  (20,000 SCF hydrogen per ton) (Reference 2), the hydrogen produced for this application is currently only about  $54 \times 10^6 \text{ std m}^3$  (0.02 TCF) annually. Worldwide direct reduction capacity as of December, 1974, was  $4.7 \times 10^9 \text{ kg/year}$  (5.2 million tons/year) with  $1.3 \times 10^9 \text{ kg/year}$  (14 million tons/year) on order.\*

\* World total steel production is  $7.1 \times 10^{11} \text{ kg/year}$  (785 million tons/year).

TABLE 2.3.3

ESTIMATED TOTAL SYNCRUDE MARKET AND SYNCRUDE CAPACITY  
BASED ON NUCLEAR-HYDROGEN PROCESSES

Year	Installed Liquefaction Capacity ( $10^{18}$ J/Year) Syncrude		Cumulative Installed Nuclear Liquefaction Capacity ( $10^{18}$ J/Year) Syncrude					
	Installed Capacity	Capacity Added Next 5 Years	1990 Entry			1995 Entry		
			5%/Yr	10%/Yr	20%/Yr	5%/Yr	10%/Yr	20%/Yr
1985	4.11		0	0	0		0	0
		4.32						
1990	8.43		0	0	0	0	0	0
		4.77						
1995	13.2		0.48	0.95	1.9	0	0	0
		5.80						
2000	19.0		2.51	5.0	7.7	0.58	1.16	2.32
		6.1						
2005	25.1		6.17	11.1	13.8	2.72	5.43	8.42
		7.6						
2010	32.7		12.6	18.7	21.4	7.28	13.0	16.0
		9.5						
2015	42.2		22.1	28.2	30.9	15.4	22.5	25.5
		11.6						
2020	53.8		33.7	39.8	42.5	27.0	34.1	37.1
		11.6						
2025	65.4		45.3	51.4	54.1	38.6	45.7	48.7
		12.6						
2030	78.0		57.9	64.0	66.7	51.2	58.3	61.3

TABLE 2.3.4

NUCLEAR HYDROGEN CAPACITY IN YEAR 2000 FOR SYNTHESIS OF SUBSTITUTE  
NATURAL GAS (SNG) AND SYNTHETIC LIQUID FUELS (SYNCRUDE)

A.D. 2000 SNG Hydrogen Requirement =  $265 \times 10^9 \text{ Std m}^3/\text{Yr}$

A.D. 2000 Liquid Fuels Hydrogen Requirement =  $642 \times 10^9 \text{ Std m}^3/\text{Yr}$

Year Nuclear Process Viable	Rate Of Market Penetration By Nuclear	SNG Market		Liquid Fuel Market (1)		Total Nuclear Hydrogen Capacity $10^9 \text{ std m}^3/\text{yr}$
		Nuclear Fraction %	Nuclear Hydrogen Capacity $10^9 \text{ std m}^3/\text{yr}$	Nuclear Fraction %	Nuclear Hydrogen Capacity $10^9 \text{ std m}^3/\text{yr}$	
1990	5%/Yr	13	34.5	13	83.5	118.0
	10%/Yr	26	68.9	26	166.9	235.8
	20%/Yr	41	106.7	41	263.2	371.9
1995	5%/Yr	3	8.0	3	19.3	27.3
	10%/Yr	6	15.9	6	38.5	54.4
	20%/Yr	12	31.8	12	77.0	108.8
2000	5%/Yr	0	0	0	0	0
	10%/Yr	0	0	0	0	0
	20%/Yr	0	0	0	0	0

(1) Includes Shale Oil



Roughly one-third of the energy requirement of a present technology steelmaking plant is in the coking coal used for reducing the iron ore, while the remaining energy is supplied as heat or electricity (Reference 8), for a total of  $1.9 \times 10^7$  J/kg ( $16.3 \times 10^6$  Btu/ton). The yield of finished steel per ton of raw steel ingot is only 69 percent; thus about  $2.7 \times 10^{10}$  J ( $26 \times 10^6$  Btu) of energy are required per 909 kg (ton) of finished steel, considering only the energy inputs to steelmaking. Most of the fossil energy is supplied today as coal.

#### 2.4.1 Market for Hydrogen in Direct-Reduction Steelmaking

The United States steel industry in 1967 consumed  $3.55 \times 10^{18}$  J (3.37 quads) or about 6 percent of the total United States energy consumption. At the projected annual growth of about 2.5 percent/year, the A.D. 2000 annual energy demand of the industry would reach  $8 \times 10^{18}$  J (7.6 quads), equivalent to the heat production of over one hundred 3000 MW(t) nuclear plants. For comparison, the year 2000 nuclear electric generation is expected to require about 1000 nuclear plants of similar size (Reference 9). The size of the market is encouraging and the energy requirements of a large steelworks fit the thermal and electric yield of a 3000 MW(t) high-temperature nuclear plant. These factors, plus growing pressure to control the pollution caused by urban-sited steel plants, favor the use of nuclear heat in steelmaking. The cost of energy for steelmaking constitutes a substantial part of the product price (manufacturing value added) (Reference 10). If the average energy cost is \$.95/GJ ( $\$1.10/10^6$  Btu), about 20 percent of the value added comes from fuel cost.

Direct reduction (DR) using natural gas is exciting worldwide interest. In the underdeveloped countries, new capacity may increasingly utilize DR, but the changeover may be slower elsewhere. As a basis of the market projection, it was assumed that the United States will have  $2.7 \times 10^{10}$  kg (29 million tons) of direct reduction steelmaking capacity installed by the year 2000. This value was used by the Bureau of Mines (Reference 2) to obtain an upper limit hydrogen projection. Table 2.4.1 develops the trend of new DR plant installations in a slightly different way, but still normalized to the Bureau of Mines estimate for the year 2000. Total United States capacity is estimated to grow at 2.5 percent per year per the usual industry projection, yielding the first two columns of Table 2.4.1. Retirements of existing plants are added in column 3 since the new capacity replacing these plants is a market also available to the DR process. A constant fraction of new plant installations is taken to be the DR type, giving new DR installations in each five-year period. These are accumulated in the fourth column. In the final column it was assumed that DR additions were twice the rate projected by the Bureau of Mines.

#### 2.4.2 Market for Nuclear Hydrogen in Direct Reduction Steelmaking

In Table 2.4.2, an estimate of how much of the DR capacity could be captured by steelmaking processes using nuclear process heat is made. If the required technology becomes commercially viable by 1990, from  $2.6$  to  $8.0 \times 10^9$  kg (2.9 to 8.8 million tons) per year of nuclear DR steelmaking capacity might be operating in 2000. A 1995 entry date is

TABLE 2.4.1

## PROJECTED STEEL PLANT CONSTRUCTION IN THE UNITED STATES

UNITS:  $10^9$  kg Steel/Year

Year	Projected Installed Capacity <sup>(1)</sup> ( $10^9$ kg)	Steel Plant Installations		Installed Direct Reduction Capacity	
		Capacity Growth In 5 Years	New Plants Installed In 5 Years <sup>(2)</sup>	Trend Fit To BOM 70 <sup>(3)</sup> Prediction For 2000	Double - BOM 70 <sup>(3)</sup> Capacity For 2000
1985	184	23	26	11	21
1990	207	27	30	15	30
1995	234	31	34	20	40
2000	265	36	39	26	52
2005	301	39	42	32	64
2010	340	45	48	38	75
2015	385	50	53	45	90
2020	435	58	61	54	101
2025	493	64	67	63	124
2030	557			73	144

(1) Based on 136 billion kg (150 million tons) in 1973, 2.5% annual growth in capacity.

(2) Includes allowance for replacement of retired units.

(3) Reference 2.

TABLE 2.4.2

ESTIMATED DIRECT REDUCTION IRONMAKING CAPACITY

BASIS: Bureau of Mines Estimate of 26 Billion kgs/Year In A.D. 2000

(Nuclear and Non-Nuclear)  
(Units: 10<sup>9</sup> kg Raw Steel/Year)

New Direct Reduction Plant Capacity Installations (BOM 70)(1)	Nuclear Steelmaking Capacity					
	Market Penetration for 1990 Entry			Market Penetration for 1995 Entry		
	Slow 5%/Year	Mod 10%/Year	Fast 20%/Year	Slow 5%/Year	Mod 10%/Year	Fast 20%/Year
1985	0	0	0	0	0	0
4						
1990	0	0	0	0	0	0
5						
1995	0.5	1.0	2.0	0	0	0
6						
2000	2.6	5.2	8.0	.6	1.2	2.4
6						
2005	6.2	11.2	14.0	2.7	5.4	8.4
6						
2010	11.3	17.2	20.0	6.3	11.4	14.4
7						
2015	18.3	24.2	27.0	12.3	18.4	21.4
9						
2020	27.3	33.2	36.0	21.3	27.4	30.4
9						
2025	36.3	42.2	45.0	30.3	36.4	39.4
10						
2030	46.3	52.2	55.0	40.3	46.4	49.4

(1) Reference 2

more likely to occur, however, resulting in only  $0.6$  to  $2.4 \times 10^9$  kg ( $0.7$  to  $2.6$  million tons)/year. These results are included in Table 2.4.3, which also shows the results of more rapid market penetrations, up to 100 percent of all new plant construction. The table indicates that in spite of optimistic assumptions, the calculated amount of nuclear hydrogen production in steelmaking processes could not exceed  $13.2 \times 10^9$  std  $m^3$  even if direct reduction processes replace competitive methods at twice the total rate implied in the Bureau of Mines estimate. For both base and high estimates, a total hydrogen demand corresponding to twice the Bureau of Mines projected DR capacity was adopted. For example, for the base number, this study takes a 1995 VHTR process and 10 percent/year penetration rate, yielding  $1.4 \times 10^9$  std  $m^3$ /year. The high estimate assumes again a 1995 process entry but a 20 percent/year penetration rate, yielding  $2.9 \times 10^9$  std  $m^3$ /year.

## 2.5 MARKET FOR HYDROGEN IN THE PRODUCTION OF AMMONIA

Since ammonia production is the principal chemical use of hydrogen, it is used here as a proxy for all chemical markets.

### 2.5.1 Present Trends in the United States Ammonia Market

Currently about  $32.2 \times 10^9$  std  $m^3$  ( $1.2$  trillion SCF) of hydrogen are consumed annually in the United States in the production of ammonia by the Haber process. About four times this may be projected for A.D. 2000. This hydrogen has not been purchased externally in the past, but was obtained by reforming natural gas (chiefly  $CH_4$ ) or naphtha.

United States ammonia production in 1973 was about  $14.5 \times 10^9$  kg ( $16 \times 10^6$  tons) (Reference 11). Production capacity is not currently increasing rapidly in the United States; the rate of increase to 1980 is projected to be only 0.7 percent (Reference 12). United States consumption, 14.3 million tons in 1973, (Reference 13), is rising at 12 percent/year. When natural gas is reformed to obtain the hydrogen for ammonia production, methane is decomposed to yield two moles of hydrogen per mole of methane, so that about 2065 std  $m^3$  (77,000 SCF) of hydrogen is required per 909 kg (ton) of ammonia. Thus, 1972 United States production amounted to  $32.2 \times 10^9$  std  $m^3$  ( $1.2 \times 10^{12}$  SCF) of hydrogen use. At 15 percent per year this could increase to  $125 \times 10^9$  std  $m^3$  ( $4.66 \times 10^{12}$  SCF) in A.D. 2000.

### 2.5.2 The World Ammonia Market

The world market for nitrogen fertilizers is increasing much more rapidly than the North American market. It is doubtful whether the United States will be able to export great quantities of ammonia, however, since the consuming countries are rapidly increasing their production capacity. Moreover, since the economics strongly favor the use of natural gas as a feedstock, the OPEC nations are in an excellent position to export fertilizer synthesized from their abundant natural gas and oil reserves. Saudi Arabia has already announced a five-year plan involving the construction of a \$5 million gas-gathering system to feed two fertilizer plants, desalination plants, and a steel mill (Reference 14).

TABLE 2.4.3  
 YEAR 2000 HYDROGEN PRODUCTION FOR DIRECT REDUCTION STEELMAKING  
 PROCESSES USING NUCLEAR-DRIVEN HYDROGEN PROCESSES

Year Nuclear Process Viable	Nuclear Penetration %/Year	Total Nuclear Steelmaking Capacity			Nuclear Hydrogen Demand <sup>(1)</sup>		
		BOM Estimate(3)	Twice BOM Est.	Limiting Case(2)	BOM Estimate (3)	Twice BOM Est.	Limiting Case(2)
		10 <sup>9</sup> kg/Year of Iron			10 <sup>9</sup> Std m <sup>3</sup> /Year of Hydrogen		
1990	5%	2.6	5.2	15.1	1.6	3.1	9.1
	10%	5.2	10.4	30.3	3.1	6.2	18.2
	20%	8.0	16.0	46.5	4.8	9.6	27.9
	33%	8.8	17.6	51.2	5.3	10.6	30.7
	100%	11.0	22	64.0	6.6	13.2	38.4
1995	5%	0.6	1.2	3.4	0.36	0.72	2.0
	10%	1.2	2.4	6.8	0.72	1.4	4.1
	20%	2.4	4.8	13.6	1.4	2.9	8.2
	33%	3.6	7.2	20.4	2.2	4.3	12.2
	100%	6.0	12	34	3.6	7.2	20.4
2000	0 - 100%	0	0	0	0	0	0

- (1) At 0.6 std m<sup>3</sup> /kg of primary iron (raw steel).  
 (2) Assuming 100% of annual steel plant additions (Table 2.4.1) are direct reduction plants.  
 (3) Reference 2

### 2.5.3 Total Hydrogen Market in Ammonia Production

Table 2.5.1 shows the total hydrogen market in fertilizer production (equated to ammonia). As a base case, it is assumed that the United States production rises at the recent trend of increase in consumption, 5.3 percent/year. This projection leads to an installed capacity in 2000 A.D. of about  $56 \times 10^9$  kg (62 million tons) per year of ammonia. At  $2.27 \text{ std m}^3/\text{kg}$  (77,000 SCF per ton) (Reference 2), the associated hydrogen demand is about  $129 \times 10^9 \text{ std m}^3/\text{year}$  (4.8 TCF/year). In the high estimate, the higher trend of world increase is used; as noted previously, it appears rather unlikely that the United States can capture much of this growing market with conventional fossil-based processes.

### 2.5.4 Market for Nuclear Hydrogen in Ammonia Production

As the basis for the assumed utilization of nuclear processes in ammonia plants, Table 2.5.2 shows the new capacity additions and various market penetration rates.

For a base nuclear projection, the 1995/10 percent per year combination is used. This amounts to a yearly nuclear hydrogen production of  $5.68 \times 10^9 \text{ std m}^3/\text{year}$ . The high estimate uses a 20 percent per year penetration rate, leading to a nuclear hydrogen use about twice as high.

The small magnitude of this hydrogen demand, computed under very optimistic assumptions, suggests that the nuclear market in ammonia and fertilizer production is relatively unimportant in 2000 A.D., but increasing rapidly thereafter.

## 2.6 MARKET FOR HYDROGEN AS A FUEL

In all of the markets discussed previously, hydrogen has already found application; indeed its use is intrinsic to synthesizing liquid or gaseous hydrocarbon fuels from coal. The position of hydrogen as a fuel itself is much more speculative. However, it is this market which has the largest ultimate potential. If all United States natural gas and SNG were replaced by hydrogen, the year 2000 demand would be  $2.8 \times 10^{12} \text{ std m}^3/\text{year}$  (105 TCF/year)\*. Even 10 percent of this market would be an enormous market for hydrogen compared to today's use.

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\* Based on 34 quads of natural gas consumption (Reference 15).

TABLE 2.5.1  
 PROJECTED A.D. 2000 HYDROGEN CAPACITY  
 REQUIRED FOR AMMONIA PRODUCTION

	$10^9$ Std m <sup>3</sup> /Year	TCF/Year
Low	67.1	2.5
Base	129	4.8
High	188	7.0

TABLE 2.5.2

POTENTIAL MARKET FOR HYDROGEN PRODUCED BY NUCLEAR  
DRIVEN PROCESS FOR AMMONIA SYNTHESIS

Year	Projected NH <sub>3</sub> Market 10 <sup>9</sup> kg NH <sub>3</sub> /Year Installed NH <sub>3</sub> Capacity      Capacity Additions In 5 Years		Nuclear Driven Hydrogen Production Capacity 10 <sup>9</sup> Std m <sup>3</sup> /Year					
			1990 Nuclear Entry Market Penetration Rate			1995 Nuclear Entry Market Penetration Rate		
			5% Year	10% Year	20% Year	5% Year	10% Year	20% Year
1973	13.9							
1985	25.8	7.6	0	0	0	0	0	0
1990	33.4	9.8	0	0	0	0	0	0
1995	43.2	12.7	2.27	4.54	8.85	0	0	0
2000	55.9	16.4	12.3	24.7	37.7	2.95	5.68	11.6
2005	72.3	21.1	34.7	62.0	74.9	15.9	31.2	48.8
2010	93.4	27.6	75.4	110	123	44.7	79.7	96.7
2015	121	36	138	173	185	97.8	142	159
2020	157	45	220	254	267	180	224	241
2025	202	60	322	356	369	282	326	343
2030	262		458	493	506	418	462	479



Potentially the largest market for hydrogen is that of a "universal fuel" supplanting conventional fossil fuels. A list of advantages often quoted for hydrogen as a fuel includes:

1. A non-polluting fuel,
2. An energy carrier with superior economics and aesthetics (using buried pipelines),
3. An effectively non-depletable energy resource if derived from nuclear or solar sources,
4. Favorable overall efficiency from resource to end use,
5. Favorable economics,
6. A storable energy form,
  - improving load-factor and hence economics of nuclear plants
  - improving reliability of energy supply to user.

Some hydrogen enthusiasts leap directly from a contemplation of these attractive qualitative characteristics to the conclusion that hydrogen is the inevitable energy carrier of the future. This kind of thinking avoids the knotty problems of how and when the United States should plan. Furthermore, statement number 3, above, has no real validity since hydrogen, like electricity is not a primary energy source.

The key to objectively determining the value of hydrogen as a fuel is to quantify its characteristics in comparison with the alternatives in each application. Although this is beyond the scope of this study, the following questions should be addressed to assess the future potential for hydrogen as a fuel in a particular application:

1. What alternatives will be available: This includes two subquestions, namely:

Will an alternative fuel technology be available to accomplish the same result?

Is the end result itself essential, or can it be replaced (e.g., if fuels for air travel become very costly, ultra high speed ground travel may replace short-haul air transport).

2. Will a hydrogen system be superior to the alternative fuel system considering the total sequence of production, delivery, and use in a specific application? "Superiority" here may denote an environmental resource conservation or economic advantage.

Note the use here of "will be" rather than "is." This study is not concerned primarily with present-day economics (which would preclude hydrogen use as a fuel), nor with competitive technologies as they exist today, but as they will exist 25, 50, and 100 years hence. Also the study cannot focus on some distant "asymptotic" future in which all fossil fuels may be imagined to be depleted, so that the question of what fuels to use reduces by default to nuclear energy as the primary source and hydrogen as an energy carrier, at least in many applications. These realities have the effect of multiplying the number of possibilities that should be considered and therefore increases uncertainties.

#### 2.6.1 Market for Nuclear Hydrogen as a Fuel

As the basis for estimating the fuel market, the total year 2000 consumption of energy for uses other than electric generation, fuel synthesis, or non-fuel uses of energy is taken. Using the pre-embargo forecast of Dupree (Reference 15) about  $1.03 \times 10^{20}$  J (98 quads) of energy in 2000 A.D. is obtained. The 1971 energy consumption in this category was  $5.02 \times 10^{19}$  J (47.6 quads). Assuming a geometric increase from this historical value, at 2.3 percent/year, additions of new fuel-using "plants" (in this case including automobiles, trains, heating furnaces, and so on) can be computed. As shown in Table 2.6.1, this will amount to about a total of  $98.2 \times 10^{18}$  J/year in the year 2000. As before, the nuclear capture of this market is estimated at several rates. Because of the scope and diversity of this sector and the lukewarm performance estimated for hydrogen in most applications except aviation, the rate of implementation is expected to be less than for the industrial uses of hydrogen. The base estimate is the 1995 nuclear system coupled with a 2 percent/year penetration of the new plant market, yielding  $0.43 \times 10^{18}$  J/year of hydrogen use in 2000 A.D., or  $33.6 \times 10^7$  std m<sup>3</sup>/year. For a high estimate, the 1995 nuclear availability entry and a 5 percent/year penetration rate, yielding  $1.08 \times 10^{18}$  J/year or  $84.4 \times 10^9$  std m<sup>3</sup>/year is used, as shown in Table 2.6.2.

#### 2.6.2 Market for Solar Hydrogen as a Fuel

In this section, consideration is given to hydrogen production by the solar-thermal, temperature gradient and wind plants, collectively describing them as solar plants. It is assumed that all solar hydrogen will be used as a fuel.

The combination of solar energy production and hydrogen as an energy carrier has a strong appeal to the ecology-minded, and continues to be much discussed by proponents of both solar power and hydrogen energy transmission.

TABLE 2.6.1

## POTENTIAL MARKET FOR NUCLEAR-DRIVEN HYDROGEN

## PRODUCTION CAPACITY AS A FUEL

UNITS:  $10^{18}$  Joules/Year

Year	Annual U. S. Non-Electric Energy Consumption		Installed Nuclear-Driven Hydrogen Capacity,								
			1990 Entry Market Penetration Rate				1995 Entry Market Penetration Rate				
			1% Year	2% Year	5% Year	10% Year	1% Year	2% Year	5% Year	10% Year	
1980	61.8		0	0	0	0	0	0	0	0	0
		7.6									
1985	69.4		0	0	0	0	0	0	0	0	0
		8.5									
1990	77.9		0	0	0	0	0	0	0	0	0
		9.5									
1995	87.4		0.19	0.38	0.95	1.9	0	0	0	0	0
		10.8									
2000	98.2		0.95	1.89	4.7	9.5	0.22	0.43	1.08	2.16	
		12.0									
20005	110.2		2.39	4.77	11.9	21.5	1.06	2.11	5.28	10.6	
		13.5									
2010	123.7		4.68	9.36	23.4	35.0	2.68	5.35	13.4	24.1	
		15.2									
2015	138.9		8.03	16.1	38.6	50.2	5.26	10.5	26.3	39.3	
		17.1									
2020	156.0		12.6	25.3	55.7	67.3	9.02	18.0	43.4	56.4	

TABLE 2.6.2  
 POSSIBLE NUCLEAR-DRIVEN HYDROGEN PRODUCTION FOR  
 USE AS A FUEL IN THE YEAR 2000

Year Technology Implemented	Rate of Hydrogen Market Penetration	Nuclear-Driven Hydrogen Production for Fuel In 2000 A D.	
		$10^{18}$ J/Yr	$10^9$ Std m <sup>3</sup> /Yr
1990	1%	.95	74.3
	2%	1.89	148
	5%	4.7	367
	10%	9.5	743
1995	1%	0.22	17.2
	2%	0.43	33.6
	5%	1.08	84.4
	10%	2.16	169
2000	0-100%	0	0

The potential for solar hydrogen production is enormous in theory. Projections of up to 0.93 billion kWh of solar electricity by 1985 and 1089 billion kWh by 2000 have been made (Reference 16). If all of this electricity were generated at 50 percent efficiency, using hydrogen from solar plants, the implied hydrogen production in the year 2000 would be  $617 \times 10^7$  std  $m^3$  (23 TCF). This type of speculation rests on two assumptions; first, that substantial solar central power will come into being by 2000 A.D. and second, that solar energy will be stored or marketed as hydrogen.

The likelihood of significant solar hydrogen production by A.D. 2000 is small since it is, in effect, the product of the probabilities that: (1) significant solar power electric generation will occur and (2) that substantial energy storage will be required and will favor hydrogen. In the near term, it is expected that energy from solar-thermal plants will be stored in the collected form; i.e., heat. For energy storage after conversion to electricity, the electrolytic hydrogen scheme must compete with a number of technologies under development. Large-scale solar hydrogen production seems especially dependent on the success of the tropic-sited sea water solar powerplant producing hydrogen as a product, a concept which will be relatively expensive to develop. If a small prototype of this plant is built in the early 1980's and a 300 MWe commercial plant by 1990, with a doubling of installed capacity in each biennium thereafter, by A.D. 2000, there would be about 30 such plants with a capacity of 9000 MWe. Assuming 50 percent efficient conversion to hydrogen, the system might produce  $1.34 \times 10^6$  std  $m^3$  (50 million SCF) of hydrogen annually. If this is increased fourfold to account for wind and other solar technologies capable of producing hydrogen, there might be  $5.3 \times 10^6$  std  $m^3$  (0.2 billion SCF) annual production of solar hydrogen by A.D. 2000. All of this hydrogen would be used as a fuel, as usually suggested by the proponents of the approach.

This study contends that the estimates cited above are overly optimistic and must be viewed as "upper-limit" estimates rather than best estimates. An estimate which is felt to represent a reasonable projection of the potential for United States solar hydrogen production is shown in Table 2.6.3.

## 2.7 MARKET FOR HYDROGEN IN OIL REFINING

This section considers both the total United States hydrogen market for oil refining and the portion of that market which nuclear processes may capture.

### 2.7.1 Projected Total Hydrogen Use in Oil Refining

With rising fossil fuel prices, refineries are increasingly using hydrogen processing techniques to increase the output of gasoline and other high hydrogen-content, high-value products. The total use of hydrogen in United States oil refining processes is projected to

TABLE 2.6.3  
PROJECTED HYDROGEN PRODUCTION USING SOLAR ENERGY

	Solar Hydrogen Production $10^9$ Std $m^3$ /Year		Annual Growth 2000-2020 %/Year
	Year 2000	Year 2020	
Low	0	0	0
Base	0.005	0.21	20
High	16.1	147.5	12

increase at a rate between 5.9 percent and 8.9 percent/year over the remaining years of this century (References 4, 17). Since the total refining capacity is increasing at only 3 percent/year, this implies that the year 2000 hydrogen use per barrel of product would be at least twice the current use of about 8 std  $m^3$  (300 SCF) per barrel

For the base estimate of hydrogen demand, a predicted consumption of 16.3 std  $m^3$  of hydrogen per barrel of oil (610 SCF/bbl) is used (Reference 2). For the assumption that the year 2000 will see an oil use, in the United States, of 13 billion barrels (Reference 15), the hydrogen demand will be  $212 \times 10^9$  std  $m^3$ /year (7.93 TCF/year). This projection implies, of course, the use of a combination of domestically produced and imported crudes.

The low estimate of hydrogen demand for oil refining reflects the consideration that our national interests may limit the United States to the use of domestically produced oil. In this case, the year 2000 oil production would be about 3.1 billion barrels per year (Reference 18). The need for hydrogen, at the same unit rate as for the base estimate, would be  $50.5 \times 10^9$  std  $m^3$  (1.89 TCF) per year.

Because of the uncertainty of oil availability and cost, and the national effort directed towards the production of synthetic liquid fuels from coal, it is imprudent to assume a high estimate for hydrogen needs in oil refining that is greater than that used for the base. Therefore, both the base and high estimates for the oil refining hydrogen market are  $212 \times 10^9$  std  $m^3$ /year (7.93 TCF/year) of hydrogen.

### 2.7.2 Nuclear Hydrogen Use in Oil Refining

The basis of the estimate of nuclear driven hydrogen production capacity for use in oil refining is shown in Table 2.7.1. New plant additions between 1985 and 2000 are assumed to equal the postulated growth plus replacement of the retired refining capacity. Beyond the year 2000, it is predicted that the need for new refining capacity disappears as synthetic fuels meet an increasing proportion of the United States energy requirements. Retirements of refining capacity will ultimately reduce the total need for hydrogen. The considerations of economics and resource management will result in the nuclear powered hydrogen processes being operated preferentially over fossil fuel driven systems.

As can be seen in Table 2.7.1, the possible penetration of the oil refining industry by nuclear processes appears to be small. This is in contrast to the production of synthetic fuels from coal, an industry which is expected to grow substantially in the same time period.

## 2.8 AREAS OF UNCERTAINTY

The emergence of the United States coal liquefaction and gasification markets depends on the attitude of private investors. A return to cheap foreign oil would threaten this capital-intensive industry. The viability of the fuel synthesis industry may thus depend on government financial backing.

The relative cost and technological maturity of hydrogen production processes as a function of time appears to be principal areas of uncertainty. The investigation, of which this market projection is a part, is well directed toward answering this problem, but further work is needed both in process design and market analysis.

One particular area of further work which could significantly improve the reliability of the market projection is the more realistic definition of the potential for the use of "merchant" hydrogen in industrial processes. To accomplish this, conceptual designs for steel-making, ammonia, and fuel synthesis plants should be made. These should consider comparable plants using "merchant" hydrogen delivered by pipeline, integrated hydrogen production/user facilities, and "conventionally" fueled plants. Using these designs and cost estimates, the market projection should be extended to derive a likely cost-benefit for each of the major hydrogen applications and a resulting potential for market penetration. Realistic rates of industry expansion in the various hydrogen-use markets should be developed with regard to rates of capital formation, foreign competition, and so on. A similar evaluation, for the purpose of better definition of the energy market for hydrogen should be undertaken. This new evaluation should include not only direct firing of hydrogen in, for example, aircraft, but the use of hydrogen as an energy storage and/or transmission medium in competition with electricity, pumped hydro storage, and synthetic hydrocarbon energy transmission systems.

TABLE 2.7.1  
 POTENTIAL MARKET FOR NUCLEAR HYDROGEN IN OIL REFINING  
 (In  $10^9$  Std Cubic Meters of  $H_2$ /Year)

Year	H <sub>2</sub> Use in Oil Refining		Cumulative Nuclear Driven Hydrogen Production for Use in Oil Refining					
			1990 Introduction Market Penetration Rate			1995 Introduction Market Penetration Rate		
	Installed Capacity	Capacity Added Next 5 Years (1)	5%/Yr	10%/Yr	20%/Yr	5%/Yr	10%/Yr	20%/Yr
1975	41.3		0	0	0	0	0	0
1985	104	28.2	0	0	0	0	0	0
1990	131	37.2	0	0	0	0	0	0
1995	167	46.2	3.72	7.44	14.9	0	0	0
2000	212	0	19.9	39.8	61.1	0	0	0
2005	212	0	19.9	39.8	61.1	4.62	9.24	18.5
2010	212	0	19.9	39.8	61.1	4.62	9.24	18.5
2015	212	0	19.9	39.8	61.1	4.82	9.24	18.5
2020	172	0	19.9	39.8	61.1	4.82	9.24	18.5
2025	137	0	19.9	39.8	61.1	4.62	9.24	18.5
2030	91	0	19.9	39.8	61.1	4.62	9.24	18.5

(1) Includes additional capacity to account for retirements.



### 3.0 SELECTION OF HYDROGEN PRODUCTION SYSTEMS FOR EVALUATION

#### 3.1 GENERAL

The selection and development of a hydrogen generation process that will have wide applicability in the period 1985 and beyond should be an important national objective. The choice of such a process should be carefully made and involve an assessment of the hydrogen production technology - both current and emerging - which will be providing the short term as well as the longer term solutions.

To conduct such an assessment, it is necessary to look not only at specific processes and their current economics, but also to factor into the analysis the required chemical feedstocks and their long-range availability. Currently, the demand for natural gas is running well ahead of supply and experts agree that this imbalance will never be corrected in the United States. Similarly, recent actions by the OPEC countries demonstrate the economic burdens wrought by ever-increasing importations of foreign oil. Consequently, the country is examining - quite properly - methods by which our abundant coal and nuclear resources might most judiciously be applied to our energy problems.

Between now and the end of the century, the world is expected to react to the fast dwindling supplies of natural gas and oil. It is believed that there will be far-reaching changes as the nation converts to a nuclear-coal energy economy. These will be accomplished by significant changes in hydrogen generation technology. Coal gasification will emerge as the dominant fossil-based hydrogen production technology, while nuclear processes which decompose water - both electrochemically and thermochemically - will arise as complementary technologies. Accordingly, the selection of hydrogen production systems will be made from the three major hydrogen production methods which will receive extensive attention to the year 2000.

The first of these, water electrolysis, will serve as a comparative baseline for the study. Since the major cost of electrolytic hydrogen is related to power costs, it is important to choose an electrolyzer capable of achieving high current densities (and therefore compact designs) while minimizing the cell driving voltage. The choice of the advanced electrolysis system, using the Teledyne Isotopes HP series modules, is discussed in Section 3.2.

The second major hydrogen production technology is based on the use of fossil fuels. Section 3.3 discusses this and presents the reasons for limiting fossil based processes to coal gasification. A preliminary assessment of the economics of hydrogen production by coal gasification involves specification of the coal feedstock, plant location and battery limits, and the purity and pressure of the product hydrogen. To be a useful planning tool, it should include not only present gasification technology, but anticipate and estimate the impact of developing technology as well. The justification for the selection of the currently available Koppers-Totzek gasification process and the developing Bi-Gas gasifier is also given in Section 3.3.

The third major hydrogen production technology is the thermochemical decomposition of water. Several water decomposition processes have been proposed in the literature and hundreds exist which have not yet been disclosed. Varying degrees of information are available on each - many are conceptual processes with no substantiating verification. Others have had some key reactions confirmed in the laboratory. None have been demonstrated on a prototype or pilot basis. Many possess serious deficiencies which would preclude their use in any large scale industrial process.

Section 3.4 discusses the technology of water decomposition and provides the basis for the selection of the Westinghouse Sulfur Cycle for evaluation. The Westinghouse process was invented to operate with a gas-cooled nuclear reactor on one side and a hydrocarbon process on the other and, as a result, it possesses interfaces compatible to both systems. The process can also provide hydrogen for other end uses. The recycling chemicals are inexpensive and substantially non-toxic, the process is capable of achieving high thermal efficiency, and a large base of applicable process technology exists to expedite process development.

## 3.2 WATER ELECTROLYSIS HYDROGEN PRODUCTION SYSTEM

### 3.2.1 State-of-the-Art

Hydrogen has been, and is, produced commercially in large quantities at low cost by the action of steam on iron or coal or by reforming hydrocarbon feedstocks. Only in areas of cheap electrical power and where large quantities of hydrogen are used locally has water electrolysis been economically justified. Smaller units, however, are attractive where the high purity (>99.8%) of electrolytic hydrogen is required. On-site hydrogen generation reduces the hazards associated with the storage of large quantities of hydrogen, saves costs associated with maintenance and resupply, and reduces dependency on outside suppliers. Available sizes range from portable units generating less than 1 liter per minute to units producing several tonnes per day.

These small production units provide the required quantities of hydrogen by employing multiples of the same basic cell, i. e., a container with an aqueous caustic solution as an electrolyte and immersed anodes and cathodes. The anodes and cathodes are separated by a diaphragm to prevent mixing of the hydrogen and oxygen produced. A schematic representation of this gas generation processes for a typical unit of a filter press electrolyzer is shown in Figure 3.2.1.

### 3.2.2 Theoretical Background

The theoretical aspects of water electrolysis can be found in a number of references (References 19, 20, 21, 22) and need not be discussed in detail. Basically, the energy required for the reaction  $\text{H}_2\text{O} (\text{liquid}) = \text{H}_2 (\text{gas}) + 1/2 \text{O}_2 (\text{gas})$  to proceed is the enthalpy of formation of water, 285.9 kJ/mole at 298K and 101.3 kPa (1 atmosphere) and corresponds to 1.482 volts/cell. Only 237.9 kJ/mole has to be supplied electrically; the remainder is required as heat and is normally supplied from electrical losses within the cell.

The energy supplied for water electrolysis is usually measured in terms of the voltage across the electrodes and the direct current passing between them. The theoretical energy is shown as a function of temperature in Figure 3.2.2. In practice, more energy is required to overcome electrode polarizations and internal resistance and is supplied as increased amperage per unit of electrode area. A ratio of the theoretical voltage to the operating voltage is a measure of the thermodynamic efficiency of the cell. The current density or amperage per unit of electrode area is a measure of the electrolysis rate or the driving force given the cell. In general, the higher the current density the lower the cell efficiency and the greater the power consumed and dissipated as heat. Theoretical and typical operating conditions are shown in Table 3.2.1.

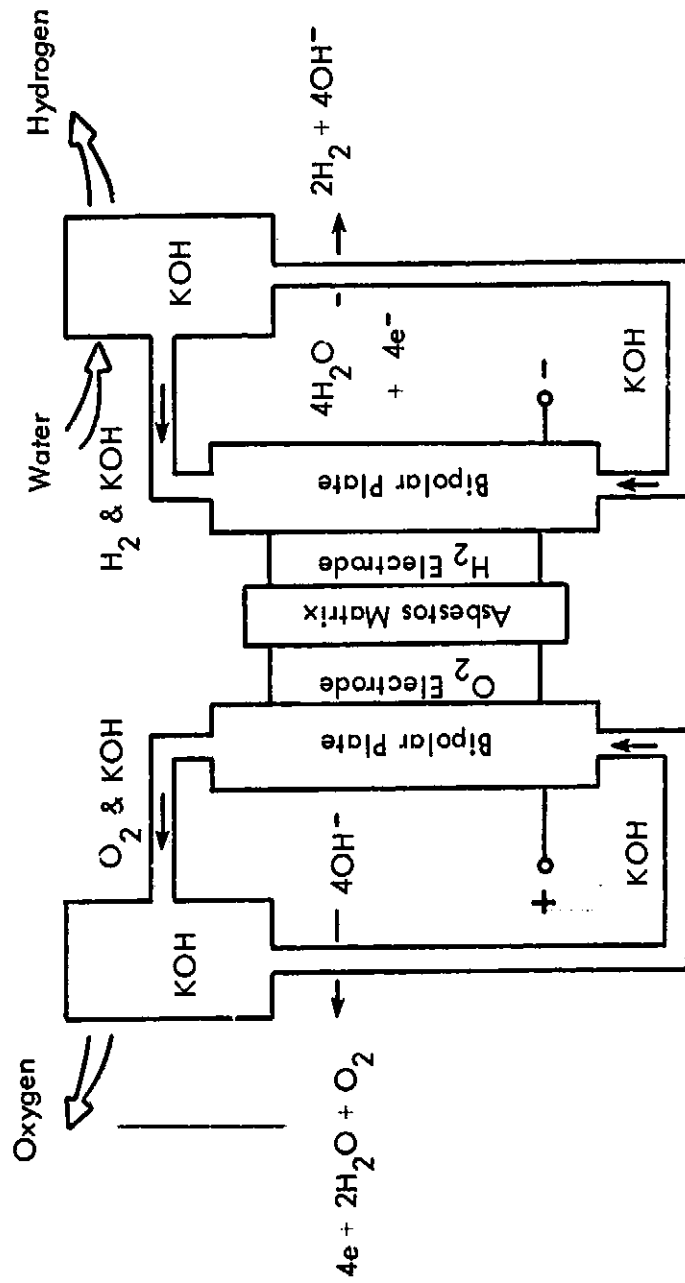


Figure 3.2.1 Schematic Representation of a Typical Unit of a Filter Press Electrolyzer  
 (Used with Permission of Teledyne Isotopes, Timonium, Maryland)

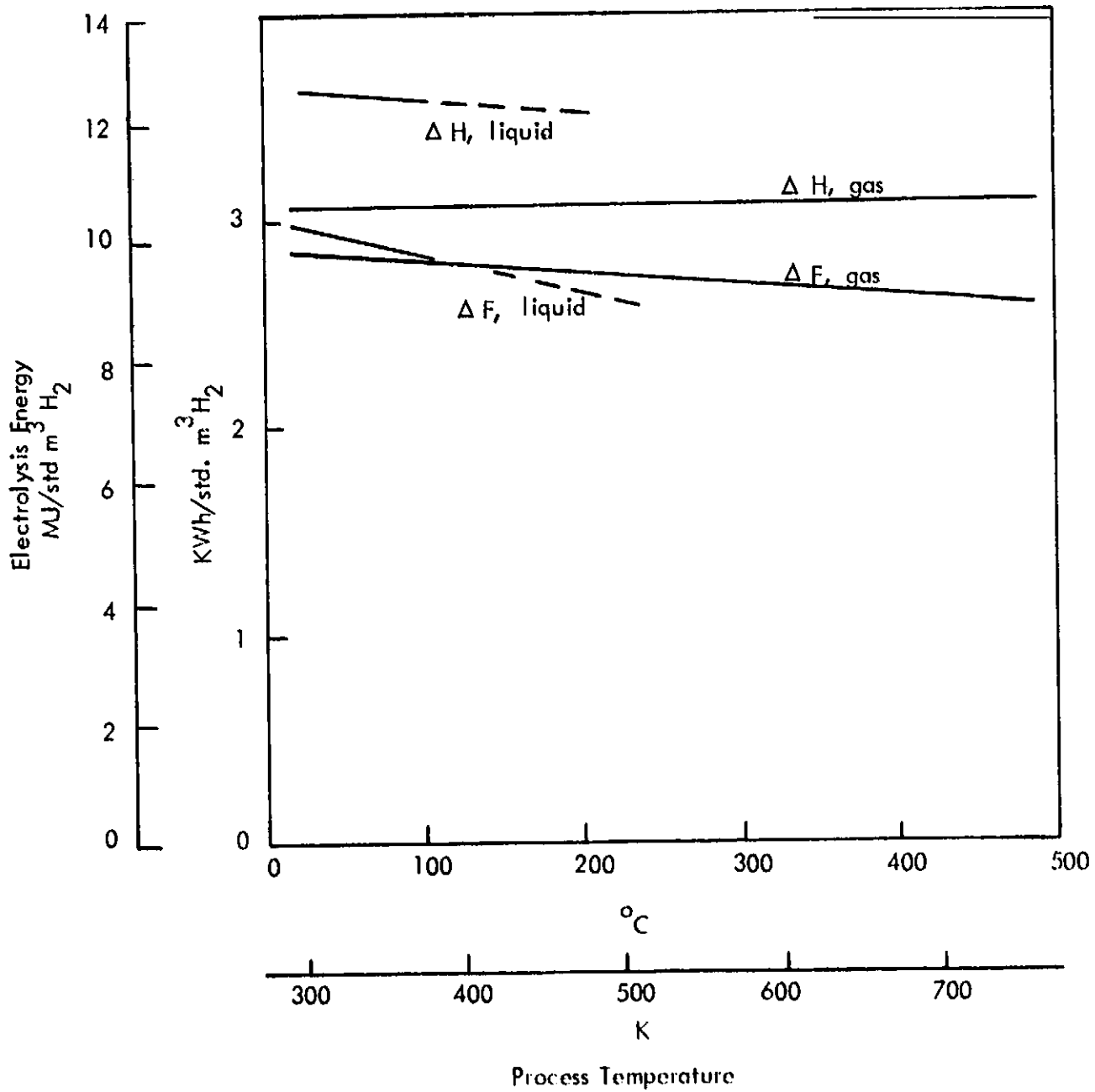
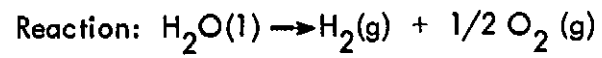


Figure 3.2.2 Theoretical Electrolysis Energy Requirements (Reference 2?)

TABLE 3.2.1  
ELECTROLYZER OPERATING CONDITIONS



	Theoretical	Typical
Temperature, K	298	348 - 358
Pressure, kPa	100	100 - 3000
Total Energy, MJ/std. m <sup>3</sup>	12.6	15.8 - 16.6
Volts/Cell	1.482	1.8 - 2.2
Current Density, ma/cm <sup>2</sup>	-	200 - 300
Overall Efficiency, %	-	50 - 65

### 3.2.3 Comparative Data on Electrolyzers

Table 3.2.2 summarizes the available information of water electrolysis equipment as compiled from several literature sources. Some fifteen suppliers of water electrolysis equipment were contacted to obtain more detailed technical and economic information on their water electrolysis systems. Seven replies were received that ranged in content from quite complete technical and economic information to a statement indicating a desire to get out of the business. Although most of the information is based on plant experience, many of orders of magnitude less than that to be treated in this report, the information received from Krebs and Company (Reference 23), Lurgi GMBH (Reference 24), Norsk-Hydro (Reference 25) and Teledyne Isotopes (Reference 26) was especially useful in the evaluation of the large scale hydrogen plant.

#### Electrolyzer Types

Electrolyzers are of either the tank-type with a series of parallel, monopolar electrodes and diaphragms hung in a tank containing the electrolyte, or the filter-press-type with bipolar electrode diaphragm assemblies compressed in series to form a module. For large scale electrolysis plants, filter press electrolyzers have an advantage because they are more compact than tank electrolyzers of the same capacity, use thinner electrodes with cells spaced to keep the quantity of circulating electrolyte at a minimum, and are more adaptable to pressurized operation. Schematic representations of these two basic types of electrolyzers are given in Figure 3.2.3.

Although filter press electrolyzers require greater quality control in manufacturing and are more expensive than tank electrolyzers, assembly line production of large numbers of modules will greatly reduce their cost. These electrolyzers usually produce hydrogen at a pressure of a few hundred millimeters of water, but a limited number of manufacturers have models that produce hydrogen at pressures of 483 kPa (70 psi) to 2102 kPa (450 psi). For a large industrial plant, electrolyzers that produce hydrogen at elevated pressures have advantages over units that produce hydrogen at pressures slightly above one atmosphere. Among these advantages are:

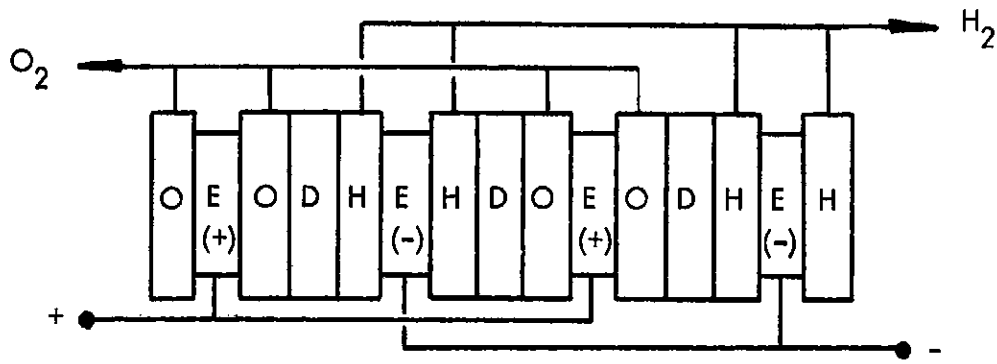
- Low specific power requirements (cell voltages decrease slightly with increasing pressure)
- Reduced compression costs
- Lower gas storage volume
- Less space required for pressurized equipment.

TABLE 3.2.2  
SUMMARY OF INFORMATION ON WATER ELECTROLYSIS EQUIPMENT<sup>(1)</sup>

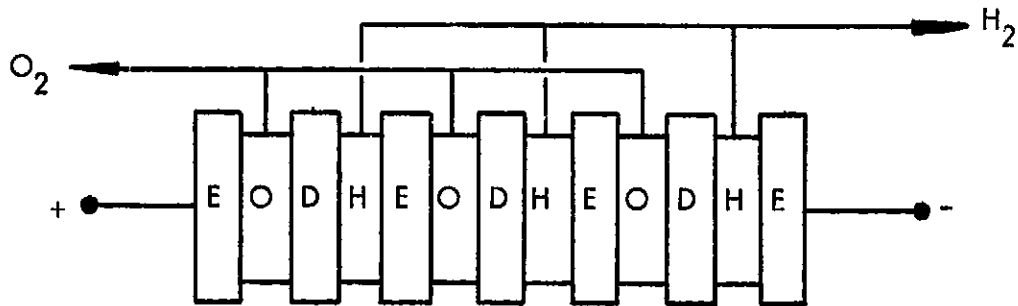
Electrolyzer Tank Type	Module Size std m <sup>3</sup> H <sub>2</sub> /h	Voltage		Current		Calculated Energy MJ/std m <sup>3</sup> H <sub>2</sub>	Pressure	
		Volts/Module	Volts/Cell	Amps/ft <sup>2</sup>	Milliamps/cm <sup>2</sup>		kPo	Atm.
<u>Cominco</u>	8.0	-	2.142	-	80	-	101	1.0
<u>Kent</u>	5.9	-	2.2	-	115	-	101	1.0
<u>Knowles</u>	5.5	-	2.0	12,000	-	15.8	101	1.0
<u>Stuart</u>	2.4	-	2.04	5,250	200	16.2	101	1.0
<u>Filter Press-Low Pressure</u>								
<u>CJB</u>	480	342	2.1	6,700	-	17.3	111	1.1
<u>Demag</u>	380	207	-	8,500	-	16.6	111	1.1
<u>DeNora</u>	861	-	2.0	-	280	16.6	111	1.1
<u>Moritz</u>	40	220	-	800	-	15.8	111	1.1
<u>Norsk-Hydro</u>	395	-	1.8	-	140	16.6	111	1.1
<u>Cerlikon</u>	210	126	-	6,600	-	14.4	111	1.1
<u>Pintsch-Bomag</u>	546	-	1.8	-	230	16.6	193	1.9
<u>Filter Press-High Pressure</u>								
<u>CJB</u>	1.4	75	-	130	-	25.2	1419	14.0
<u>Teledyne HP</u>	525	440	1.8	5,210	200	15.8	689	6.8
<u>Teledyne Adv. HP</u>	525	385	-	5,210	-	13.7	689	6.8
<u>Teledyne HS</u>	12.0	375	-	200	-	22.7	689	6.8
<u>Treccwell O<sub>2</sub> Gen.</u>	6.8	55	-	1,050	-	30.6	20270	200.0
<u>Zdarsky-Lanza</u>	882	-	1.8	-	200	16.6	3040	30.0

<sup>(1)</sup> References 19, 23, 24, 25, 26, 27





(a) Tank-type, Mono-polar



(b) Filter-press type, Bi-polar

E = Electrode

D = Diaphragm

H = Hydrogen

O = Oxygen

Figure 3.2.3 Schematic Comparison of Tank and Filter-Press Electrolyzers

### Power Requirements

The power requirements for the electrolyzer plant of the size considered is in the order of 2000 MWe. If an electrical generation thermal efficiency of 30 to 40 percent is assumed, powerplants of from 5000 MWt to 6000 MWt are foreseen. For long term economic reasons the powerplants will probably be nuclear units. Because of the large power consumption of water electrolysis plants, the environmental impact of the power generation facilities should be assessed against the electrolytic hydrogen plant.

### Feedwater Requirements

The electrolyzers require high quality feedwater at a rate of 0.85 to 0.90 liters/std  $m^3$   $H_2$ . For a  $9.6 \times 10^6$  std  $m^3$   $H_2$ /day ( $360 \times 10^6$  SCFD) production plant, this amounts to 350  $m^3$ /hour 1540 gallons/min). This water is first processed in a water pre-treatment plant to a purity almost equivalent to heating steam condensate. The water is further purified by distillation or deionization (current trends lean toward deionization) to specific resistances ranging from  $>50,000$  ohm-cm to 1 megohm-cm. The water should be free of chloride, sulfate, and metal ions and have  $<4$  ppm dissolved solids and  $<1$  ppm suspended solids.

### Cooling Water Requirements

Power losses due to ohmic resistances in the electrolyzer produce waste heat that is removed from the circulating electrolyte by cooling water. Water is also used to cool the hydrogen and oxygen streams. Cooling water utilization ranges between 30 liters/std  $m^3$   $H_2$  to 50 liters/std  $m^3$   $H_2$  with inlet temperatures around 293K. For a  $9.6 \times 10^6$  std  $m^3$   $H_2$ /day ( $360 \times 10^6$  SCFD) hydrogen plant, this amounts to between 11,500  $m^3$ /hour to 19,200  $m^3$ /hour (50,000 to 85,000 gallons/min) of cooling water.

### Electrolyte Preparation

The electrolyte is prepared from good quality sodium or potassium hydroxide. Although potassium hydroxide is more expensive and shows a more rapid attack upon materials of construction, a 25 percent KOH solution is the preferred electrolyte for filter press electrolyzers not only because of its higher conductivity, but also because of the lower vapor pressure of the solution. Purchase specifications state that the potassium hydroxide be 87 - 90 percent chemically pure (the bulk of the impurity is water) with maximum concentrations of impurities specified as follows:

$K_2CO_3 < 0.5\%$ ,  $KCl < 0.1\%$ ,  $K_2SO_4 < 0.1\%$ , and other metal ions-nil.

The initial filling of the electrolyzer and associated systems for the production of  $9.6 \times 10^6$  std  $m^3$ /day ( $360 \times 10^6$  SCFD) requires the dilution of about  $5 \times 10^6$  Kg ( $11 \times 10^6$  lbs) of potassium hydroxide with processed feedwater (specific resistance 75,000 ohm cm) to a 25 w/o caustic potash solution. A nitrogen blanket is advised during electrolyte preparation, initial charging, and start-up to prevent  $CO_2$  absorption from the air.

TABLE 3.2.3

## TYPICAL MATERIALS USED IN WATER ELECTROLYZERS

Item	Material
Bus Bars	Copper
Cell Frames	Teflon Coated Steel
Electrodes	Nickel or Nickel Plated Steel
Diaphragms	Asbestos
Vessels, (Separators, Heat Exchangers, etc.)	Stainless Steel
Piping	Stainless Steel
Seals	Halogenated Hydrocarbon Polymers
Demister Filters	Sulfuric Acid, Silica Gel, or Alumina

### Electrolyte Circulation

The electrolyte is heated and maintained at operating temperatures of 353 to 363K. It is circulated through the cells, heat exchangers, and filters to maintain a constant operating temperature, reduce polarization effects due to bubble formation and concentration gradients, and to remove suspended solids ( $K_2CO_3$ ) and possible corrosion products).

### Electrolyzers

Current cell and system designs require little maintenance and operate at relatively high efficiency for long periods of time. For example, normal corrosion and contamination of the cell may cause a reduction of current efficiency from 98 percent at startup to about 96 percent after 6 - 8 years of operation. Routine maintenance consists of changing filters, repairing minor leaks, and correcting instrumentation faults.

### Safety

Every effort is made to prevent explosive mixtures of hydrogen with oxygen or air from occurring and to avoid hot spots or electric sparks where hydrogen is present. This requires isolation of electrical equipment from the cells, good electrical insulation, explosion proof motors and pumps, and good seals to prevent electrolyte leakage that could lead to electrically conducting crystalline hydroxide deposits.

Compact electrolyzer designs minimize the amount of hazardous material present at any given time. Individual cells (less than 2 cm in cross section to about 180 cm in diameter) consist of nickel plated steel electrodes separated into anode and cathode compartments by reinforced asbestos diaphragms. These diaphragms, if they are neither stretched nor allowed to dry out, operate satisfactorily for more than ten years. However, should they rupture to cause intermixing of hydrogen and oxygen or should hydrogen leak into a confined air space or should a line blockage occur, various devices (pressure relief valves, alarms, interlocks, automatic shut-offs, nitrogen purges, etc.) are present to prevent or limit any damage that may occur. In addition, pipelines are present to vent the gases to the atmosphere if a potentially hazardous condition develops. Cell power will also be terminated, and reactions in the cells would cease.

### Hydrogen

After separation from the entrained electrolyte, the water saturated hydrogen stream has a nominal purity (dry basis) of  $99.8 \pm 0.22$  percent. The major impurity is oxygen; and, if necessary, the oxygen can be removed by a "deoxo" catalyst, and the hydrogen can be dried to a lower dew point.

Typical analyses of product hydrogen streams are shown in Table 3.2.4.

TABLE 3.2.4

## HYDROGEN PRODUCT STREAM ANALYSIS

Electrolyzer	Hydrogen Product Stream		
	Pressure	Moisture	Purity (Dry Basis)
Zdansky-Lonza (LURGI)*	3000 kPa	Saturated	99.9 vol% H <sub>2</sub> 0.1 vol% O <sub>2</sub> <0.1 mg KOH/std.m <sup>3</sup>
Demag (KREBS)*	≥ 100 kPa	Saturated	99.8 vol% H <sub>2</sub> 2-5 mg KOH/std. m <sup>3</sup>
I.S Series (Teledyne)**	600 kPa	188K Dew Point	0.05-0.2 ppm O <sub>2</sub> 0.01-0.1 ppm H <sub>2</sub> O 0.1-0.2 ppm HC as CH <sub>4</sub> 0.05-0.2 ppm N <sub>2</sub> <0.1 ppm CO <0.05 ppm CO <sub>2</sub> 4 ppm total impurities

\* After electrolyzer, condenser, and trap

\*\* After condenser, trap, molecular sieve, and submicron filter

### Oxygen

Although the hydrogen stream is to be compressed to 6895 kPa (1000 psi) and piped to an off-site user for consumption, the oxygen stream is considered to have no value and is vented to the atmosphere. After separation from the entrained electrolyte, the water saturated oxygen stream has a nominal purity (dry basis) of 99.5 ± 0.3 %. The major impurity is hydrogen.

Typical analyses of the oxygen streams are shown in Table 3.2.5.

TABLE 3.2.5  
OXYGEN PRODUCT STREAM ANALYSES

Electrolyzer	Oxygen Stream		
	Pressure	Moisture	Purity (dry basis)
Zdansky-Lonza (LURGI)*	3000 kPa	Saturated	99.4 vol% O <sub>2</sub> 0.6 vol% H <sub>2</sub> <0.1 mg KOH/std m <sup>3</sup> O <sub>2</sub>
Demag (KREBS)*	≥ 100 kPa	Saturated	99.5 vol% O <sub>2</sub> 50-70 mg KOH/std m <sup>3</sup> O <sub>2</sub>
HS Series (Teledyne)**	600 kPa	188 K Dew Point	< 4 ppm total impurities (assume same types and relative amounts as shown for hydrogen)

\*After electrolyzer, condenser, and trap

\*\* After condenser, trap, molecular sieve, and submicron filter.

The most likely place in the process for venting the oxygen stream is after the condenser and trap so that the pure water feed and electrolyte carried over from the main gas-electrolyte separation can be recovered and recycled. The level at which KOH emission becomes a pollutant will determine if gas velocity and a suitable stack height results in sufficient dispersion and dilution of the stream or if gas filtration is needed before venting to the atmosphere.

#### 3.2.4 Environmental Constraints

Although water electrolysis is essentially a "clean" process, a plant producing  $9.6 \times 10^6$  std m<sup>3</sup>/day ( $360 \times 10^6$  SCFD) of hydrogen will have some impact on the environment. The most significant impact is that of the power generation facilities required to support a hydrogen plant of this large size. A 5000 to 6000 MWt powerplant is required, and environmental concern will be a factor in siting the plant and selecting the mode of power generation. The second most significant impact is that of the large cooling water demand of from 11,000 to 12,000 m<sup>3</sup>/hour. If it is assumed that the cooling water will be recycled through cooling towers, make-up water requirements drop, but the environmental impact of the cooling

towers have to be considered. The third most significant item is the continual discharge of large quantities of oxygen saturated with water vapor and possibly containing potassium hydroxide as a trace contaminant. Other items such as feedwater treatment plant chemicals, solid waste disposal, etc., would be no more than the norm for any light duty industrial plant of comparable size.

### 3.2.5 Water Electrolysis Plants

The largest hydrogen plants use the standard filter-press electrolyzers and are the 1,434,000 std m<sup>3</sup>/day plant at Rjukan, Norway using Hydro-Pechkrantz cells (Norsk-Hydro) and the 894,000 std m<sup>3</sup>/day plant at Aswan Dam, Egypt, using Demag cells (Krebs and Co.). It is of interest to note that the plant size basis for this report (9,600,000 std m<sup>3</sup>/day) is almost seven times larger than the largest hydrogen plant using standard filter press electrolyzers.

Some the advantages in using a pressurized water electrolyzer for a large scale industrial hydrogen plant were given earlier in this section. At present, the only large capacity pressurized water electrolyzer available is the Zdansky-Lonza Electrolytor (LURGI-GMBH). The Zdansky-Lonza modules produce hydrogen at 3000 kPa (about 425 psi) with a specific energy requirement of 15.5 to 16.6 MJ/std m<sup>3</sup>H<sub>2</sub>. More than 30 units have been build to date with an overall capacity exceeding 450,000 std. m<sup>3</sup>/day. The largest module size is about 21,000 std. m<sup>3</sup>/day, and the largest plant size is about 110,000 std. m<sup>3</sup>/day. The plant size basis for this report is almost 90 times larger than the largest hydrogen plant using pressurized water electrolyzers.

Teledyne Isotopes is currently manufacturing commercial 690 kPa (100 psi) hydrogen generators in sizes up to 200 standard liters per minute (HS Series) and has extended this technology to the design of larger plants (HP Series). A pilot module will begin operation in mid-1975 and produce hydrogen at 690 kPa with a specific energy requirement representative of current commercial technology of about 15.8 MJ/std. m<sup>3</sup>H<sub>2</sub>. An advanced HP series cell operating at about 13.7 MJ/std. m<sup>3</sup>H<sub>2</sub> has been demonstrated in the laboratory, and Teledyne expects that it will become commercially practical in the near term (1980-1985).

### 3.2.6 Electrolyzer Selection

Of the several types of electrolyzers commercially available, pressurized filter press electrolyzers have been selected for the conceptual development of a large hydrogen plant because they are compact, have less internal hold-up of hydrogen, occupy less floor space for a given volume of hydrogen, produce a pure hydrogen stream that requires less

compression for pipeline delivery, are cost competitive with standard filter press electrolyzers, and have a greater potential for future improvements. Pressure electrolyzers are available in module capacities up to 2.2 tonnes/day. To represent the technology of pressure electrolyzers, the HP modules of Teledyne Isotopes were selected. Teledyne currently markets small pressure electrolyzers and has a prototype 1.75 tonne/day module scheduled for operation in mid-75. Information provided by Teledyne indicated that the HP modules were competitive in both performance and price to electrolyzers produced by others.



### 3.3 FOSSIL BASED HYDROGEN PRODUCTION PROCESSES

#### 3.3.1 General

Fossil based hydrogen production encompasses processes which employ reactions of steam and hydrocarbons. These processes are:

- Steam-hydrocarbon reforming for operation with gaseous feedstocks such as methane, ethane, naphtha, etc.
- Partial oxidation for use with liquid feedstocks such as heavy and residual oils.
- Coal gasification.

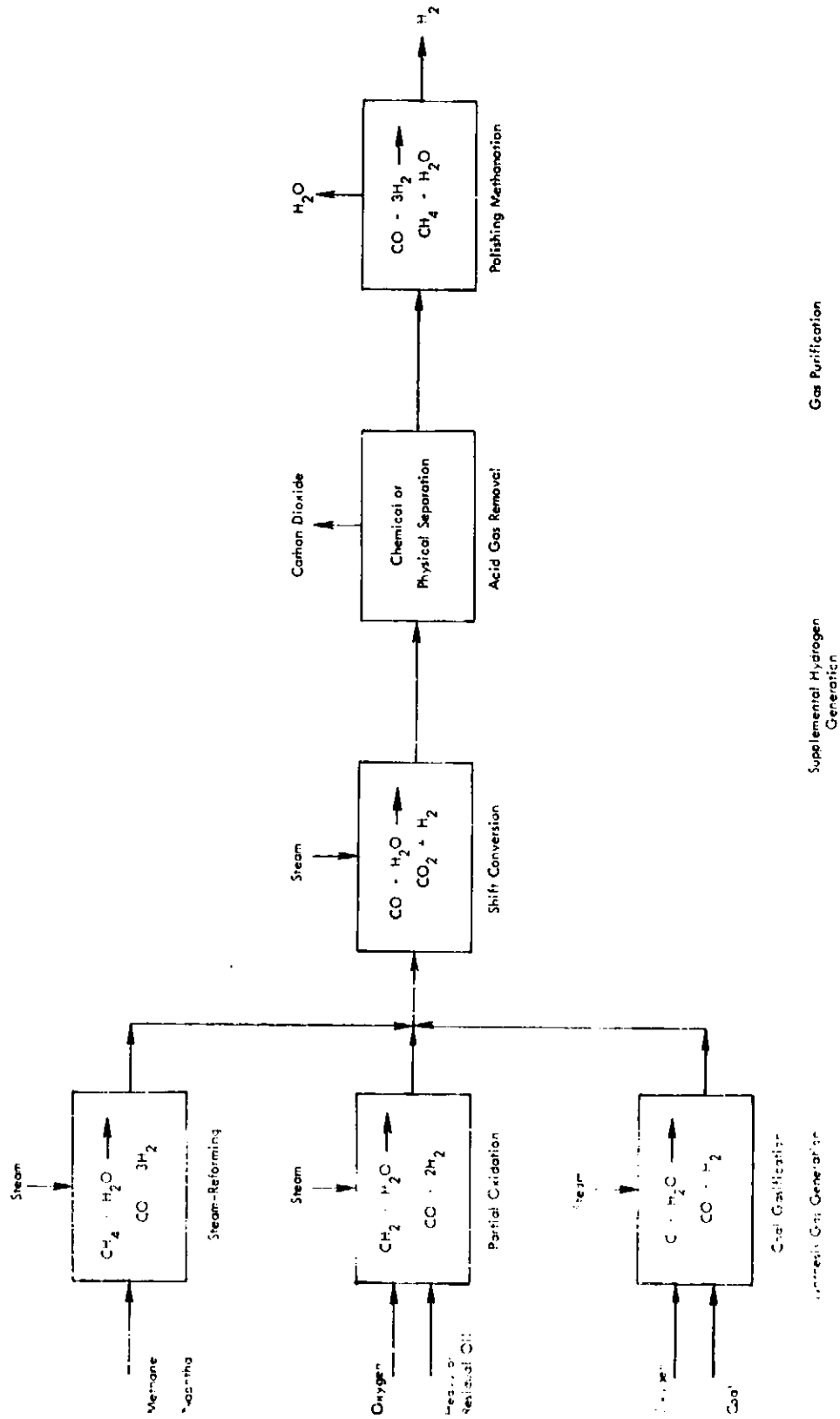
Steam-hydrocarbon reforming designates processes which employ a gaseous feedstock such as methane, ethane, naphtha, or similar light hydrocarbons. Partial oxidation processes are those which use a liquid feedstock such as heavy or residual oil, and gasification refers to processes operating with a solid feedstock such as coal, coke, char, and perhaps municipal or process waste. In general, chemical reactors designed for one primary feedstock are not readily converted to another. For example, a steam-methane reformer cannot be used to conduct coal gasification reactions, nor can a coal gasifier be used effectively as a methane reformer. Similarly, within each group, the chemical reactor and its operation will depend upon the physical and chemical properties of the feedstock. Not all coal gasifiers, for example, can accommodate caking or agglomerating coals, and all gasifiers require some degree of coal preparation and sizing prior to gasification. For all steam-hydrocarbon processes, steam and fuel requirements vary with feedstock, as does the nature and the duty of downstream processing.

Figure 3.3.1 shows, schematically, the three basic fossil based methods for generating hydrogen, including the typical downstream processing steps incorporated to provide a high purity hydrogen product stream. Polishing methanation is used to rid the product stream of any contained carbon monoxide.

The selection of the fossil based hydrogen generation processes to be evaluated for applicability in the years 1985 and beyond, in comparison to water electrolysis and thermochemical water decomposition, must be carefully done and involve an assessment of hydrogen production technology - both current and emerging - which will be providing the short term as well as the long term solutions. It is also necessary to look not only at the specific process and its current economics, but also to factor into the analysis the required chemical feedstocks and their long-range availability.

#### 3.3.2 Selection of Type of Fossil Based Hydrogen Production System to be Studied

Technology currently exists, and new technology is being developed, to permit any of the three generic types of fossil based production systems, i.e., steam reforming, partial



Supplemental Hydrogen Generation

Gas Purification

Figure 3.3.1 Fossil-Based Methods for Generating Hydrogen

oxidation, and coal gasification, to be applied to the goal of meeting the future needs for hydrogen. The choice of type, therefore, has to be made on a basis other than that of technology. It becomes readily apparent, then, that the cost of the produced hydrogen, taking into account the capital investment and the cost and availability of fossil feedstocks, will be the chief rationale by which a selection is made.

Until recently, methane at the well-head was available for less than 37.9¢/GJ (40¢/10<sup>6</sup> Btu). This feedstock cost, coupled with the lower capital investment required for reforming plants, made steam-methane reforming the preferred hydrogen generation process. Methane availability, as natural gas, is no longer assured, and significant escalation of its price is expected. As a result, intensified interest has been shown in partial oxidation and coal gasification processes for hydrogen production.

With present oil prices, and the economic burdens placed on the nation by the ever-increasing importation of foreign oil, it does not appear that partial oxidation will be able to capture major new U. S. markets, particularly if the feedstock is derived from natural crudes. Synthetic crude oil can be obtained, however, from coal liquefaction processes presently under development. This syncrude represents a potential feedstock for use in partial oxidation systems.

Numerous cost estimates have been prepared detailing coal liquefaction economics. For example, the H-Coal process is capable of producing a \$50.3/m<sup>3</sup> (\$8/bbl) Syncrude from a 37.9¢/GJ (40¢/10<sup>6</sup> Btu) coal (Reference 28). If one were to compare the production costs of direct gasification of the coal and subsequent processing of the synthesis gas to hydrogen to the production of syncrude from coal followed by partial oxidation to obtain hydrogen, the more economical hydrogen production process would be coal gasification.

Therefore, looking to the future, it is probable that processes which employ the partial oxidation of heavy oil for large scale hydrogen generation will not be competitive with other steam-hydrocarbon systems. Partial oxidation processes could not be based upon domestic crude, as long term contracts can no longer be obtained. If based upon foreign crudes, the hydrogen price would be economically unattractive. Operating with a syncrude derived from coal liquefaction, the partial oxidation process does not compete with coal gasification.

A similar situation exists with respect to steam-methane reforming. The feedstock employed in the process can be derived either from natural sources or from coal gasification processes presently being developed. The cost of producing SNG (synthetic natural gas) from coal is also well-documented. Using a 37.9¢/GJ (40¢/10<sup>6</sup> Btu) coal produces a SNG product at \$1.66/GJ (\$1.75/10<sup>6</sup> Btu) (Reference 29).

As in the case of partial oxidation, the cost of hydrogen produced from an appropriate coal gasification process can be compared to the cost of hydrogen produced by reforming the SNG obtained from coal. Once again, coal gasification is the more economical process.

The results summarized above are general, but lead to the conclusion that synthetic oil and synthetic gas obtained from coal will be too expensive to justify its use in any large scale hydrogen production facility. As a result, the viability and long-term feasibility of the partial oxidation and steam-methane reforming processes must be based upon their economics when processing natural, rather than synthetic, feedstocks. Because of the short fall in natural gas supply, the limitations in domestic crude production, and the economic burden of imported oil, these processes for hydrogen production cannot be considered suitable to meet the needs of the future. Therefore, it is concluded that coal gasification will emerge as the dominant fossil-based hydrogen generation technology of the future. For the purpose of comparative evaluation with electrolytic and thermochemical hydrogen generation systems, then, only coal gasification processes are used to represent the contribution of fossil fuels to hydrogen production.

### 3.3.3 Coal Gasification Systems

With the attention being given to coal gasification development programs within the United States today, it is easy to forget that gasification has been practiced industrially for over fifty years. Commercial coal gasifiers can be purchased from a variety of vendors, and additional gasifiers and processes will soon be available as a result of industrial and ERDA-sponsored programs.

In order to provide useful information for evaluation purposes, it is believed to be important to assess the technology for producing hydrogen by two coal gasification processes. One of these would involve gasifiers currently available today, and thus would reflect the gasification economics pertinent to plants operating in the late 70's and early 80's. The second would be based upon gasifiers presently under development, and would reflect the economics of middle 1990's operation.

Currently, gas producers are available commercially in one of three major gasifier types: fixed-bed, fluidized-bed, and entrained-flow or suspension types. Representative sketches of each type are shown in Figures 3.3.2, 3.3.3, and 3.3.4. For hydrogen manufacture, each producer would be oxygen-blown, and would have reaction zones at some point in the gasifier at temperatures in excess of 1144K (1600°F). It should be noted that none of these producers is readily amenable to indirect heating and that heat exchange surface within any of these refractory-lined, water-jacketed vessels would be exposed to an extremely hostile environment. Therefore, none of these coal gasification options could consider a nuclear heat source in the technical and economic evaluation.

For a given coal, the synthesis gas produced by each of these generators will be different, due to different pressures of operation as well as different overall temperature distributions throughout the producer. The selection of a gasification process for hydrogen generation thus involves first the selection of the gasification pressure and secondly the choice of a gasifier type. Trade-offs are involved in both selections. Gasification under pressure has the advantages that:

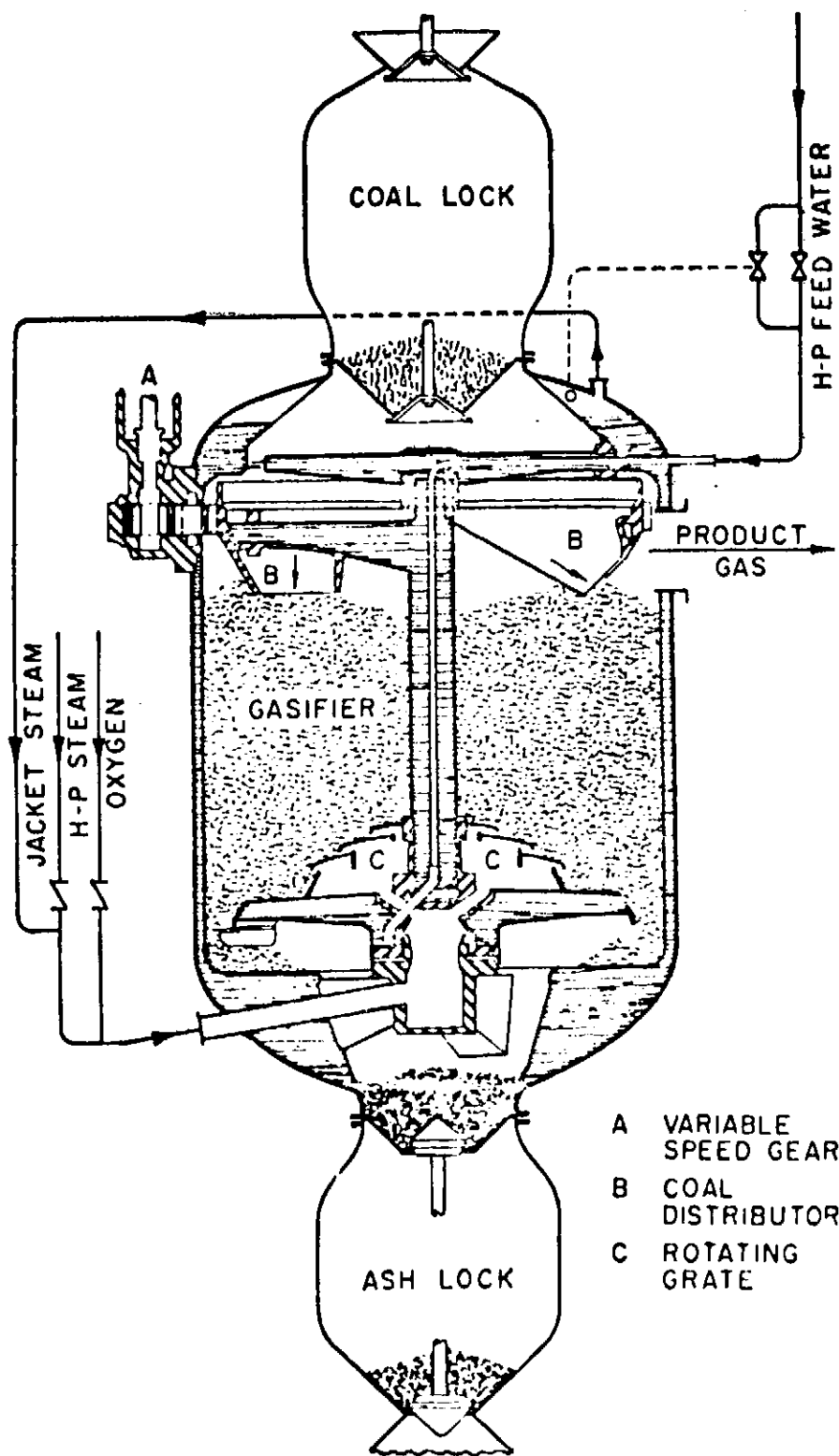
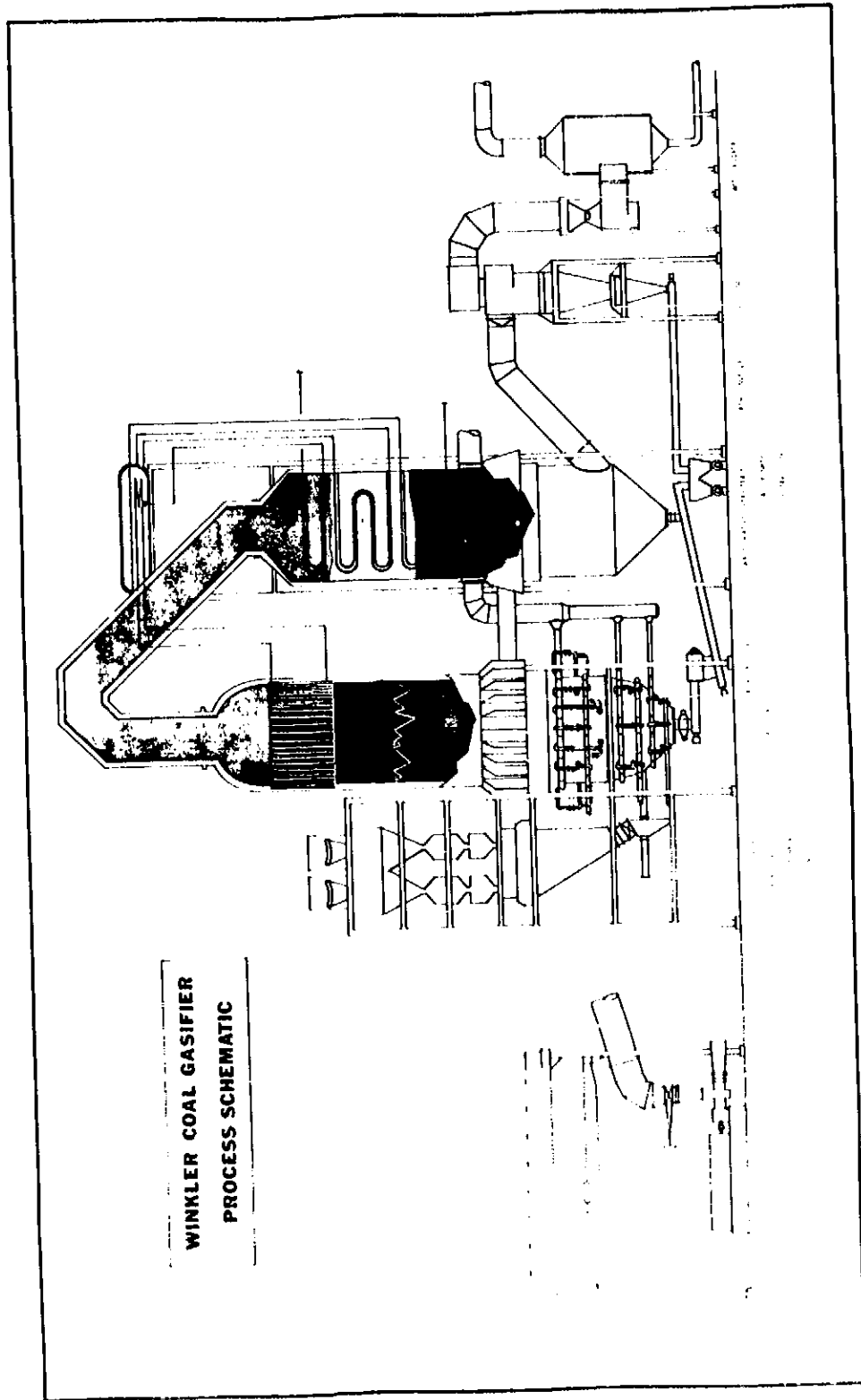


Figure 3.3.2 Fixed-Bed (Lurgi)



**WINKLER COAL GASIFIER  
PROCESS SCHEMATIC**

Figure 3.3.3 Fluidized-Bed (Winkler)

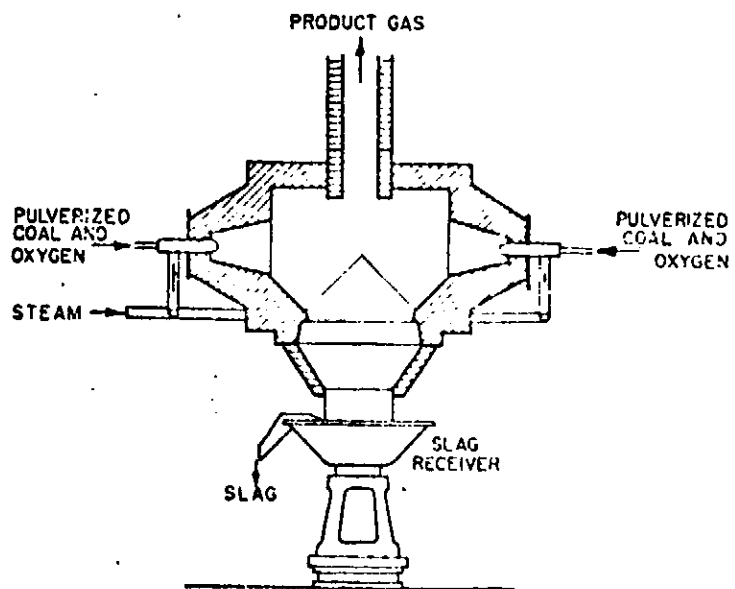


Figure 3.3.4 Entrained (Koppers-Totzek)

- Higher gasification rates (due to higher reactant partial pressures) are achieved.
- Compression costs are minimized for those applications where pressurized gases are required, e.g., transmission pipelines, ammonia production.
- Smaller vessels are required for downstream processing units.
- Higher gas densities lead to higher heat transfer rates.

Gasification under pressure possesses some disadvantages. These include:

- Methane must be removed if high purity hydrogen is required.
- The direct production of CO rich gases (desirable for hydrogen manufacture) requires the use of slagging processes.
- Coal must be fed into and ash removed from a pressurized vessel.
- Some coals which are noncaking at atmospheric pressure become caking at higher pressures.

Similarly there are advantages and disadvantages inherent in the use of a particular gasifier type. These are summarized below.

#### Fixed-Bed Gasifiers

<u>Advantages</u>	<u>Disadvantages</u>
● Countercurrent movement of solids and gases leads to high heat economy	● Caking coals require pretreatment
● Long solid residence time produces high carbon conversion efficiencies	● Sized fuels are necessary
	● Tars are produced at the top of the bed and must be removed if the gas is to produce high purity hydrogen
	● Higher methane yields are obtained



### Fluidized-Bed Gasifiers

#### Advantages

- Gasification rates are higher than those obtained in fixed-beds
- Operation over a wide range of conditions is possible without significant losses in efficiency
- High inventory of fuel prevents oxygen breakthrough

#### Disadvantages

- High loss of sensible heat in the exit gas
- High loss of ungasified coal in exit gas
- Large ash contents in the bed are necessary to avoid significant carbon losses in the underflow
- Slugging and other maldistributions of gas and solids can occur
- Fluidization characteristics of the fuel limit the operating conditions of the system

### Entrained (Suspension Gasifiers)

#### Advantages

- Any grade or class of coal can be used
- Gasification rates are the highest of any of the three gasifier types
- Product gas contains no tar and little, if any methane
- Wide range of operating conditions is possible
- Readily adaptable for pressurized and slagging operation

#### Disadvantages

- High carbon conversions require recycle of solid residue
- Heat exchange is necessary to improve thermal efficiency

In selecting a gasifier type for a hydrogen production process, it should be recognized that gasifiers well-suited to methane production are not particularly appropriate for hydrogen manufacture and vice versa. Most of the gasification processes under development

today employ pressurized gasifiers of the fixed-bed and fluidized-bed types. Included in this category are the Lurgi, Synthane, Hydrane, IGT, and CO<sub>2</sub> Acceptor Processes. These processes, by operating at lower temperatures and higher pressures, encourage maximum methane formation in the gasifier. Higher overall heat economies and process thermal efficiencies are achieved, leading additionally to lower oxygen consumptions and less shift conversion and acid gas removal capacity. All of these factors contribute to more favorable process economics if methane is the desired product.

Entrained gasifiers, on the other hand, while not as well suited for methane production, produce a synthesis gas free of tars, and low in methane. Such gas is ideally suited for hydrogen, ammonia, methanol and Fischer-Tropsch synthesis. Such gasifiers possess the additional advantages of being able to handle all coals, without pretreatment, and are capable of achieving high gasification rates.

In evaluating the economics of producing hydrogen by coal gasification, these differences become important. For instance, the Lurgi gasifier (a fixed-bed producer) - which operates at lower temperatures and pressures of about 2000 kPa (20 atm) - achieves excellent heat economy. The Koppers-Totzek gasifier (an entrained-flow gasifier) operates at about 100 kPa (one atm) and high temperatures and achieves poorer heat economy. This leads to a more expensive synthesis gas compared to that obtained from Lurgi gasification and more downstream compression is required. Use of this more expensive gas may be justified, however, as it is a much better feedstock for hydrogen manufacture than is the Lurgi gas. Reference to Table 3.3.1 shows that the Koppers-Totzek gas is essentially CO + H<sub>2</sub> with negligible amounts of methane and higher hydrocarbons. Thus, after shift conversion and acid gas removal (Table 3.3.2) this gas is capable of producing much purer hydrogen.

Whether this is an advantage or a disadvantage depends upon the application. If (formation) pressures of 6895 to 13790 kPa (1000 to 2000 psi) are required and the presence of methane is not detrimental. The Lurgi gas would probably be the preferred feedstock in this, and in applications involving initial coal hydrogenation in liquefaction processes, as well as fuel applications. If the gas is to be used in hydrotreating hydrocarbon liquids, methanol synthesis, fuel cells, or similar high purity applications, the Koppers-Totzek gas is preferable.

For the purpose of the technical and economic evaluation, it is concluded that the advantages of the entrained gasifiers in respect to the purity of hydrogen produced makes the results of the evaluation more directly comparable to the results from processes producing hydrogen by electrolytic means. Therefore, two gasification processes - both employing suspension gasifiers - will be assessed. The first of these will be the Koppers-Totzek gasifier and a process designed to produce hydrogen at a purity of at least 95 percent and a pressure of 6895 kPa (1000 psia). The evaluation of this system will provide an assessment of the cost of producing high purity hydrogen using current technology.

The second gasification process will employ the Bi-Gas gasifier being developed by Bituminous Coal Research. This gasifier is presently in the pilot stage at BCR's facility

TABLE 3.3.1  
TYPICAL RAW GASES FROM LURGI AND KOPPERS-TOTZEK  
GASIFIERS FOR COMPARABLE BITUMINOUS COALS

<u>Component</u>	<u>Lurgi Gasifier</u>	<u>Koppers-Totzek Gasifier</u>
CO <sub>2</sub> + H <sub>2</sub> S	32.2	9.2
C <sub>n</sub> H <sub>m</sub>	0.2	-
CO	16.3	53.0
H <sub>2</sub>	39.3	36.4
CH <sub>4</sub>	11.3	-
N <sub>2</sub>	0.4	1.1
H <sub>2</sub> O	0.3	0.3
TOTAL	100.0	100.0

TABLE 3.3.2  
DRY GAS ANALYSIS AFTER SHIFT CONVERSION AND ACID GAS REMOVAL

<u>Component</u>	<u>Lurgi Gasifier</u>	<u>Koppers-Totzek Gas</u>
C <sub>n</sub> H <sub>m</sub>	0.3	-
CO	Nominal	Nominal
H <sub>2</sub>	82.8	98.8
CH <sub>4</sub>	16.3	-
N <sub>2</sub>	0.6	1.2
TOTAL	100.0	100.0

in Homer City, Pennsylvania. The synthesis gas is available at 6895 kPa (1000 psia), thereby avoiding compression costs. The high pressure encourages some methane formation, but due to the slagging-suspension design, not as much as that obtained from other systems being developed. The Bi-Gas system, however, due to advanced design, produces higher pressures and lower tar levels, while simultaneously providing the benefits of suspension gasification. These include higher throughputs per unit and ability to operate with all coals, both caking and non-caking.

Conducting the gasification technical and economic assessment in this fashion provides information on the performance and the cost of hydrogen production by gasification as a function of high or low pressure gasification and existing or developing gasifiers.

### 3.4 WATER DECOMPOSITION HYDROGEN PRODUCTION SYSTEMS

Water decomposition hydrogen production processes, as used here, are those processes in which water is used as a feedstock and, through thermochemical or combined thermochemical-electrolysis reactions, is dissociated to form hydrogen and oxygen. A characteristic of this class of hydrogen production processes is that the thermochemical reactions are cyclic in nature, i.e., the chemical intermediates are recovered and reused. Water decomposition processes employing only electrolysis are excluded from this category of hydrogen production systems and considered as a separate class of processes, as discussed in Section 3.2.

In principle, water can be decomposed thermally in a single step. Extremely high temperatures are necessary to achieve significant degrees of dissociation and effective separation of the hydrogen/oxygen mixture is required. By employing a series of reactions involving cyclic intermediates, the maximum temperature necessary for decomposing water can be significantly reduced. Several such "water-splitting" processes have been proposed and many are under active investigation in laboratories around the world. Section 3.4.2 compares the characteristics of representative systems. Inherent in all of these systems is the desire to maximize thermal efficiency, minimize overall (including power generation) capital investment, and utilize chemical reactions which can be demonstrated to occur.

All water splitting processes, due to their cyclic nature, are Carnot-limited. As a result, the overall process thermal efficiency depends upon both the maximum temperature one can obtain from the thermal source driving the process and the particular series of chemical reactions employed in the water decomposition sequence. The maximum thermodynamic process thermal efficiency is represented by the equation (Reference 30).

$$\eta_M = \min. \left\{ \begin{array}{l} \frac{\Delta H^\circ}{\Delta G^\circ} \\ 1.0 \end{array} \cdot \frac{T_H - T_C}{T_H} \right\}, \text{ where}$$

- $\eta_M$  = Maximum thermal efficiency
- $\Delta H^\circ$  = Heat of formation of water at 298K
- $\Delta G^\circ$  = Free energy of water at 298K
- $T_H$  = Heat source temperature
- $T_C$  = Heat sink temperature

Table 3.4.1 shows the maximum thermal efficiency as a function of heat source temperature. As indicated, with heat sources above 1089K (1500°F) available, water splitting process efficiencies theoretically equivalent to those for fossil-based processes are possible.

TABLE 3.4.1

MAXIMUM THERMAL EFFICIENCY OF WATER DECOMPOSITION PROCESSES

<u>Heat Source Temperature</u>		<u>Maximum Thermal Efficiency, %</u>
<u>K</u>	<u>°F</u>	
800	980	75.3
900	1160	80.3
1000	1340	84.4
1100	1520	87.7
1200	1700	90.4
1300	1880	92.7
1400	2060	94.7

Water splitting processes assume particular importance when methods are sought for generating hydrogen from indirect sources of heat, particularly that available from either high temperature gas-cooled nuclear reactors or from solar collectors. Hydrogen is more easily stored and transported than thermal energy. Significant markets for hydrogen and oxygen will be created as plants for converting coal into synthetic oil and gas go onstream. If this hydrogen can be obtained from other than fossil-based processes, our ultimate reserves of fossil fuels can be prolonged.

Hydrogen obtained from water splitting processes can similarly be expected to be important in nuclear process heat applications, especially those involved with substituting nuclear heat for coal in coal conversion systems. The substitution of nuclear for fossil energy in a fossil-based hydrogen production system is limited by the chemical characteristics of the process. A certain portion of the hydrocarbon feedstock is consumed in chemical reactions; the balance in meeting the process heat requirements. Only the latter may be substituted. Water splitting processes enable complete substitution and enable a single hydrogen production process to be employed, regardless of energy source.

3.4.1 Water Splitting Processes as a Class § Hydrogen Generation Methods

A variety of methods exist for producing hydrogen. As hydrogen is not a primary energy form, its synthesis, in all instances, requires the addition of more primary energy than

is subsequently recovered during hydrogen combustion. Depending upon the form of the primary (or secondary energy), the method of hydrogen production may vary. Steam-hydrocarbon reforming designates processes which employ a gaseous feedstock such as methane, ethane, naphtha, or similar light hydrocarbons. Partial oxidation processes are those which use a liquid feedstock such as heavy or residual oil, and gasification refers to processes operating with a solid feedstock such as coal, coke, char, and perhaps municipal or process waste. In general, chemical reactors designed for one primary feedstock are not readily converted to another. For example, a steam-methane reformer cannot be used to conduct coal gasification reactions, nor can a coal gasifier be used effectively as a methane reformer. Similarly, within each group, the chemical reactor and its operation will depend upon the physical and chemical properties of the feedstock. Not all coal gasifiers, for example, can accommodate caking or agglomerating coals, and all gasifiers require some degree of coal preparation and sizing prior to gasification. For all steam-hydrocarbon processes, steam and fuel requirements vary with feedstock, as does the nature and the duty of downstream processing. Electrolysis characterizes those processes employing electrical energy, as DC power, to electrolytically decompose water into hydrogen and oxygen. Water splitting processes similarly decompose water, but employ a series of chemical reactions involving cyclic chemical intermediates to decompose water at temperatures well below its thermal decomposition temperature.

While electrolysis and water splitting are clearly water decomposition processes - each using a form of energy to produce hydrogen and oxygen from water - it is important to note that the conventional steam - hydrocarbon processes for hydrogen production are in reality water decomposition systems as well.

Consider, as an example, the gasification of carbon with steam to produce a synthesis gas for hydrogen production. The gasification reaction is



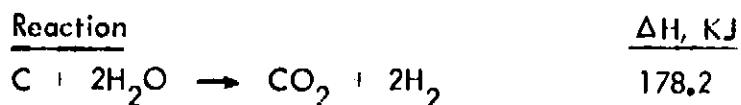
This is followed by the water gas-shift reaction



so that the total process is represented as



Overall, Reaction 3 is endothermic by 178.2 KJ, thus for an ideal process, the energy balance shown below applies



Thermal Inputs

Carbon Heating Value	393.5
Endothermic Reaction Heat	178.2
Total	571.7

Comparing this with the thermal requirements of an ideal water decomposition process illustrates the similarities and differences in the two methods of hydrogen production.

Coal Gasification

<u>Reaction</u>	<u><math>\Delta H</math>, KJ</u>
$C + 2H_2O \rightarrow CO_2 + 2H_2$	178.2

Thermal Inputs

Coal Heating Value	393.5
Endothermic Reaction Heat	178.2
Total	571.7

Water Decomposition

<u>Reaction</u>	<u><math>\Delta H</math>, KJ</u>
$2H_2O \rightarrow 2H_2 + O_2$	571.7

Thermal Inputs

Water Heating Value	0
Endothermic Reaction Heat	571.7
Total	571.7

A similar situation exists with regard to steam methane reforming. In this case, the energy balances shown below apply.

Steam Methane Reforming

<u>Reaction</u>	<u><math>\Delta H</math>, KJ</u>
$0.5CH_4 + H_2O \rightarrow 0.5CO_2 + 2H_2$	126.5

Thermal Inputs

0.5 mole $CH_4$	445.2
Process Heat	126.5
Total	571.7

Water Decomposition

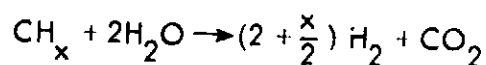
<u>Reaction</u>	<u><math>\Delta H</math>, KJ</u>
$2H_2O \rightarrow 2H_2 + O_2$	571.7

Thermal Inputs

$2H_2O$	0
Process Heat	571.7
Total	571.7



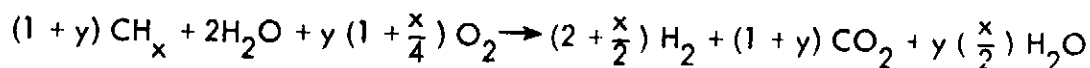
The mass and energy balances illustrated earlier show that coal gasification and steam methane reforming are specific methods by which hydrocarbons may be used to decompose water in order to obtain hydrogen. The results are general, since in all cases the overall process reaction is given by



The heat of reaction is  $\Delta H_{\text{rxn}} = \Delta H_{\text{CO}_2} - 2 \Delta H_{\text{H}_2\text{O}} - \Delta H_{\text{CH}_x}$  where  $\Delta H_i$  is the heat of formation of compound  $i$  from the elements at the reference temperature. The process thermal inputs are:

Heating Value of $\text{CH}_x$	$\Delta H_{\text{CH}_x} - \Delta H_{\text{CO}_2} - (\frac{x}{2}) \Delta H_{\text{H}_2\text{O}}$
Reaction Enthalpy	$\Delta H_{\text{CO}_2} - 2 \Delta H_{\text{H}_2\text{O}} - \Delta H_{\text{CH}_x}$
Total	$-(2 + \frac{x}{2}) \Delta H_{\text{H}_2\text{O}}$

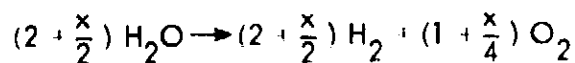
As the total balance shows, the process energy inputs as reactants and fuel will always be identical to those which would have been required had water been decomposed directly. When hydrocarbon fuels are burned to meet the process energy needs, the overall mass balance becomes



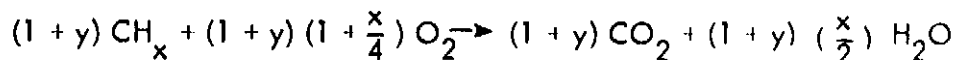
where

$$y = \frac{\Delta H_{\text{CO}_2} - 2 \Delta H_{\text{H}_2\text{O}} - \Delta H_{\text{CH}_x}}{\Delta H_{\text{CH}_x} - \Delta H_{\text{CO}_2} - (\frac{x}{2}) \Delta H_{\text{H}_2\text{O}}}$$

A water decomposition process operating on the same fuel at the same thermal efficiency would accomplish the reaction



by combusting the fuel in air to drive the process. From combustion one has



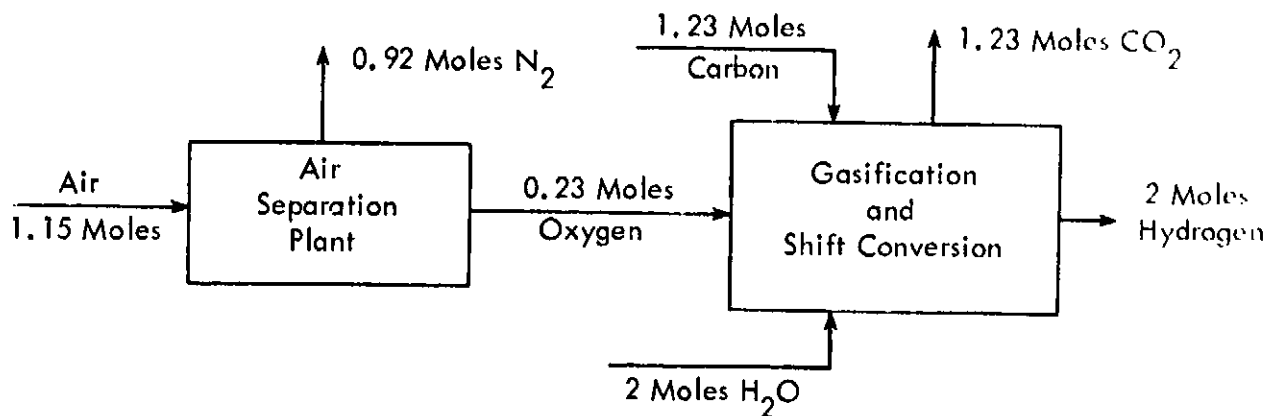
As the net mass balances for the process indicate, overall fuel and water consumption remain unchanged. The water decomposition process, however, has the advantage of being able to provide oxygen as well as hydrogen.

Two major differences exist between water decomposition and steam-hydrocarbon processes for hydrogen generation. The first relates to the amount of process energy which can be supplied by non-fossil means. For the steam-hydrocarbon processes, less than 25 percent of the theoretical energy requirements can be substituted with non-fossil energy sources. The balance of the hydrocarbon is consumed as a chemical reactant, not as a process fuel. In practice, due to process inefficiencies, much larger fractions of the hydrocarbon feedstock are devoted to fuel usage and thus larger portions are potentially available for substitution.

Reductions in the quantities of hydrocarbons required to produce hydrogen can be achieved in any of three ways. Non-fossil energy can be substituted for that portion of the fossil feedstock which is consumed as fuel, efforts can be taken to improve the efficiency of the hydrogen generation process; or efficient processes independent of hydrocarbon feedstocks can be developed. While fuel substitution within existing processes and improvements in overall thermal efficiency are worthwhile, it is important to note that all three methods of reduction can be achieved with the water-splitting processes.

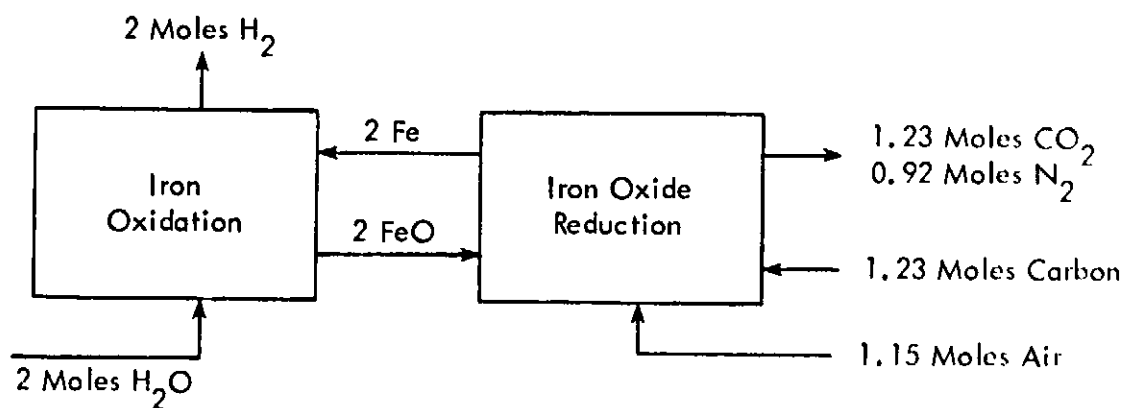
The second major difference between water splitting and steam-hydrocarbon is the by-product formed during hydrogen generation. Both processes operate with the same total thermal inputs yet one produces a useful by-product, oxygen, while the other does not. The primary reason for this difference rests with the partitioning of reactants and fuels within the process. Considering the case of coal gasification, it is theoretically possible (at one hundred percent thermal efficiency) to obtain 2 moles of hydrogen by reacting 1.23 moles of carbon with 2 moles of water and at least 1.15 moles of air. Depending upon the equipment configuration, either the process will require an oxygen plant, or it will avoid the need for an oxygen plant, or it will act as though it is simultaneously an oxygen plant.

It is instructive to consider three processes by which hydrogen may theoretically be obtained from carbon and water. The first involves the use of oxygen-blown gasification followed by shift conversion. Assuming an ideal process, the mass balances shown below will apply.

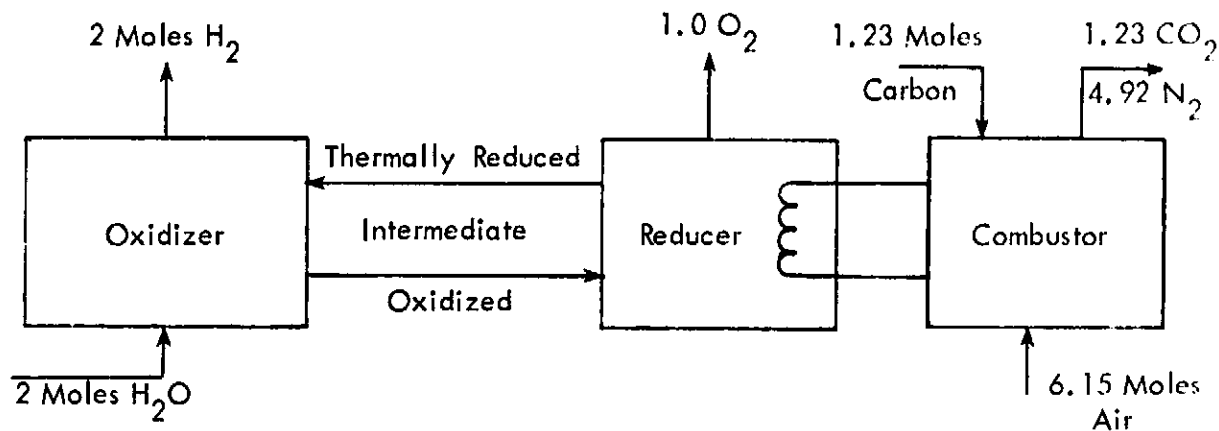


The fact that carbon is being oxidized in the same vessel that is being used to conduct the hydrogen generation reaction requires an oxygen plant to prevent dilution of the product gas with nitrogen. If the hydrogen generating reaction can be separated from the major endothermic process reaction, then air rather than oxygen can be used in fueling the process.

This is the approach used when hydrogen is generated using a steam-iron process. In this instance, again assuming an ideal process, the mass balances shown below apply.



In its simplest form, a thermochemical process for decomposing water is similar to an indirectly heated steam-iron process. For an ideal process, the mass balances shown below apply.



Compared with the steam iron process, 1.15 moles of air are required to combust 0.23 moles of carbon for process heat. The remaining five moles are effectively separated into four moles of nitrogen which are vented and a mole of oxygen which is recovered.

Notice also, by adding carbon to the reduction step of the thermochemical process for decomposing water, that it theoretically becomes equivalent to the steam-iron process. Similarly, indirect heating of iron oxide to liberate oxygen would make this equivalent to a thermochemical process. As the energy balances show, 109.6 MJ (103,827 BTU) must be expended to decompose a mole of water vapor into hydrogen and oxygen. Mass and energy balances for a carbon-fueled process indicate that at least 1.23 moles of carbon and 1.15 moles of air are necessary. Processes can be devised to meet these mass and energy requirements in different ways.

The use of a single reaction vessel requires an oxygen plant to prevent dilution of the product gas with nitrogen and fails to recover the oxygen for subsequent utilization. The use of two primary reaction vessels is sufficient to avoid the use of oxygen and enables the process to employ air instead. Firing one process vessel directly with carbon and air potentially leads to higher thermal efficiencies, but also fails to recover the oxygen byproduct. Indirectly firing the second vessel, while perhaps lowering the thermal efficiency, enables both decomposition products to be recovered for utilization.

Additional advantages are obtained by using the water decomposition process. The most important of these is the fact that hydrogen can be generated from any convenient fuel, e.g., coal, oil, gas, nuclear, or solar. For each of the hydrocarbon processes, an unique fossil fuel/feedstock requirement is evident. The potential of substitution of one energy form for another is limited.

In the case of steam-methane reforming, methane equivalent to 200 MJ/kg-mole (86,080 Btu/lb-mole) hydrogen must be provided as a chemical reactant. In principle, only an additional .085 moles  $CH_4$ /mole  $H_2$  is required for the process heat requirement. Even allowing the possibility of substitution, a sizeable methane requirement remains. For the

water decomposition process, however, the most economic energy source - whatever it may be - can be used by modifying that equipment through which the energy is transmitted to the process. This energy can be provided as either methane, oil, coal, nuclear, solar, or any combination of sources to result in the most economical hydrogen production. This feature will be of ever increasing importance in the decades to come, as the cost and availability of various fuels and feedstocks vary with economic conditions and energy reserves.

#### 3.4.2 Basis of Selecting a Water Decomposition System

The selection of a water decomposition process is complicated by the large number of such cycles under study and the generally limited data available on each. Several water decomposition processes have been proposed in the literature and hundreds exist which have not been disclosed. Varying degrees of information are available - many are conceptual processes with no substantiating experimental verification. Others have had some of the key reactions confirmed in the laboratory. None have been demonstrated on a prototype or pilot basis. Many of these cycles have been invented during the course of Government-funded research, and, as a result, are available for analysis and review. Others were developed privately and the supporting information has not been published.

While the task of devising cycles is relatively simple - one organization, using a computer, has generated over 5000 candidate processes - not all of these will be applicable as hydrogen sources for industrial uses. Many possess serious deficiencies which would preclude their use in any large scale industrial process. Often the primary reactions in the sequence do not proceed at economical rates, or methods have not been devised to avoid complicating side reactions. Frequently exotic chemicals are employed, a fact which would ultimately limit the number of commercial installations possible before chemical reserves would be depleted. Many of the theoretically more efficient cycles are required to deliver major portions of the total process energy at temperatures above 1144K (1600°F) and often to solids. These pose heat transfer and chemical reactor design problems requiring imaginative, and perhaps expensive solutions.

The ideal thermochemical cycle for water decomposition is one which minimizes product cost by achieving high thermal efficiencies in a process with low capital and operating costs. The efficiency should be maintained over a range of heat source temperatures, thereby permitting maximum flexibility in the choice of energy sources and heat exchanger materials.

The nature of the chemical cycle affects capital costs in several ways. Hopefully simple, compact chemical reactors can be employed. This necessitates choosing reactions which proceed rapidly and without serious side reactions occurring. Separation of reactants and products should be simple. Reaction reversals at lower temperatures may require elaborate quench and separation systems.

The presence of noxious impurities in the hydrogen and oxygen product streams may necessitate expensive cleanup facilities to meet health or environmental requirements. Similarly losses, and perhaps degradation, of the recycling chemicals will occur, and depending upon the process, may adversely affect operating cost.

Lacking process flowsheets and kinetic data on key reactions in a thermochemical cycle, it is impossible to prepare even preliminary capital and operating cost estimates. However, for a given thermochemical cycle, it is at least possible to provide some preliminary estimates on maximum thermal efficiency and minimum operating cost. Similarly it is possible to comment, at least initially, on the feasibility of reactions employed in the cycle and whether serious competing reactions might occur.

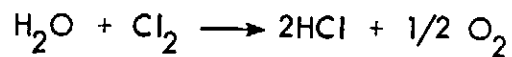
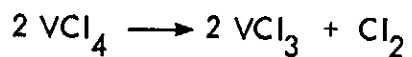
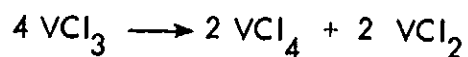
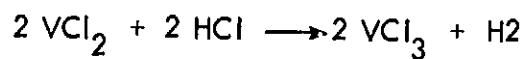
A total of eighteen published processes advocated by ten different organizations have been evaluated using a series of prescreening criteria. These are summarized in Table 3.4.2. The first phase of the evaluation procedure recognized that losses of the recycling chemical intermediates will occur and attempts to estimate the impact of these losses on the process operating costs. In practice, these losses can occur in various ways. Leaks and blowdowns are inherent in all chemical processes. No separation process removes all of the secondary component. Hydrogen and oxygen leaving the process must either be of exceptionally high purity or else carry with it small quantities of the intermediate chemicals. The presence of only 500 ppm of intermediate in each of the two product streams is sufficient to require the make-up of 0.1 percent of the recycling inventory.

The first phase of the evaluation procedure assesses the feasibility of the chemicals proposed for use in the cycle. This assessment is conducted by considering a water decomposition process which produces  $13.4 \times 10^6$  standard  $m^3$  ( $500 \times 10^6$  SCFD) hydrogen and  $9.6 \times 10^6$  Kg/day (10,600 TSD) oxygen. This corresponds to what is believed will be a typical installation with a 4000 MWt nuclear heat source and the water splitting cycle operating at a thermal efficiency of about 50 percent. The chemical recycle rate in the process is assumed to be stoichiometric and the loss of 0.1 percent of the recycle rate is assumed for each recycling chemical. This provides a reasonable set of assumptions for determining the operating cost associated with make-up chemicals for the process. Table 3.4.3 shows, for each of the eighteen processes, the chemical consumption and cost as calculated. Clearly high thermal efficiency is of diminishing value if exotic chemicals must be employed, as the gains achieved by lower nuclear fuel consumption are offset by the make-up chemical cost. A maximum tolerable chemical cost adder of 9.47  $\text{¢/GJ}$  ( $10\text{¢}/10^6$  Btu) was considered as a threshold for economic viability. Beyond this point, improvements in efficiency are largely negated by chemical costs. The results of this chemical make-up cost screening are summarized in Table 3.4.4. As indicated, only eight of the eighteen cycles possess operating costs sufficiently low to warrant further study.

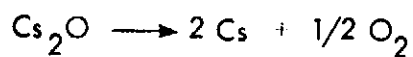
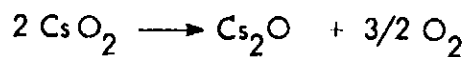
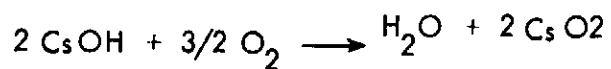
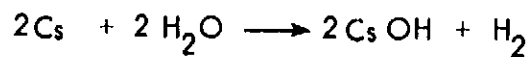
TABLE 3.4.2

THERMOCHEMICAL WATER DECOMPOSITION PROCESSES  
CONSIDERED FOR HYDROGEN GENERATION

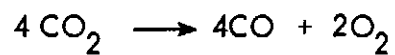
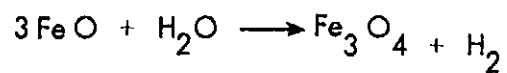
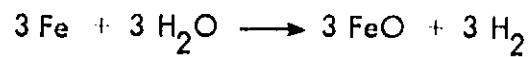
PROCESS NUMBER 1: Vanadium Chloride Cycle  
Allison Division - General Motors  
Funk and Reinstrom



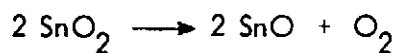
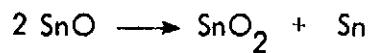
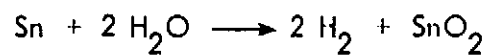
PROCESS NUMBER 2: Cesium Oxide  
Aerojet General  
Miller and Jaffe



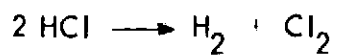
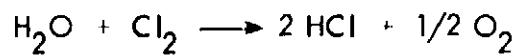
PROCESS NUMBER 3: Steam-Iron-Carbon Dioxide  
Institute of Gas Technology  
von Fredersdorff



PROCESS NUMBER 4: Tin Oxide  
Gaz de France  
Souriau

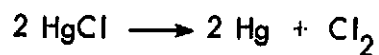
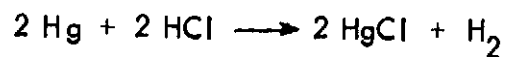
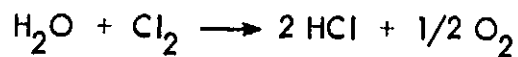


PROCESS NUMBER 5: Hydrogen Chloride Electrolysis  
Air Products  
Hallett

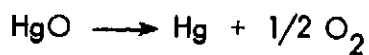
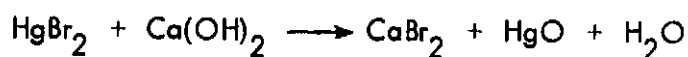
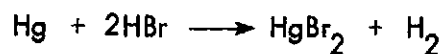
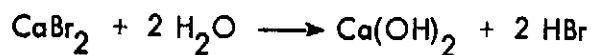




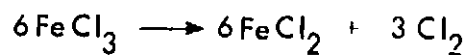
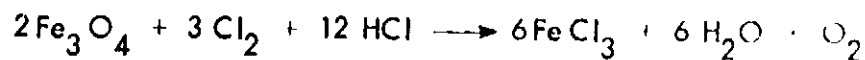
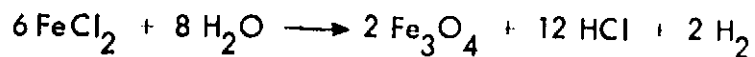
PROCESS NUMBER 6: Mercury Chloride Electrolysis  
Institute of Gas Technology  
Gregory



PROCESS NUMBER 7: Euratom Mark-1  
Euratom  
Marchetti and deBeni

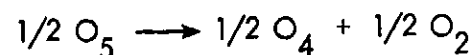
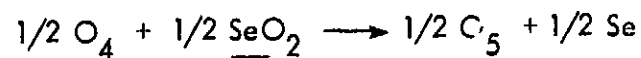
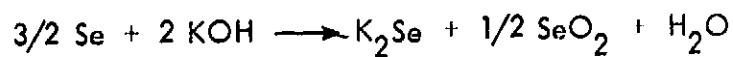
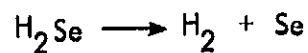
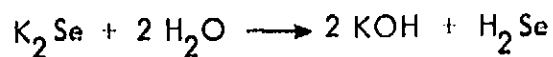


PROCESS NUMBER 8: Euratom Mark-9  
Euratom  
Hardy



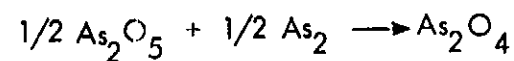
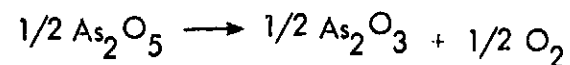
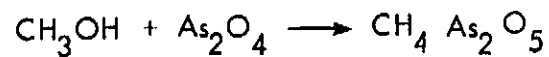
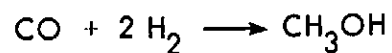
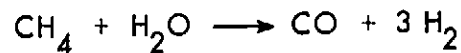
PROCESS NUMBER 9:

Selenium Cycle  
Lawrence Livermore Laboratory  
Hickman, Kriforian, and Ramsey

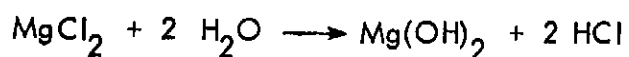
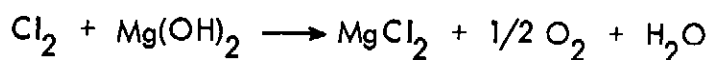
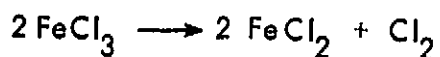
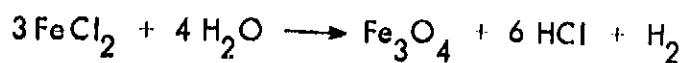


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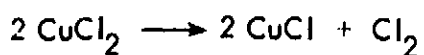
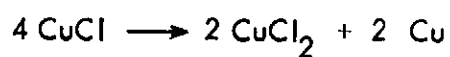
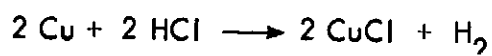
Methane-Methanol Cycle  
Lawrence Livermore Laboratory  
Hickman, Krikorian, and Ramsey



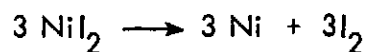
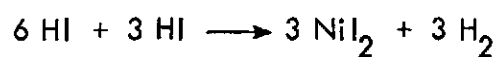
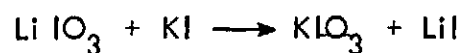
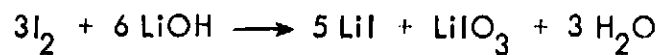
PROCESS NUMBER 11: Agnes  
General Electric  
Wenford and Hanneman



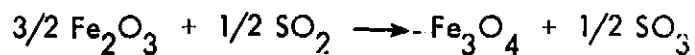
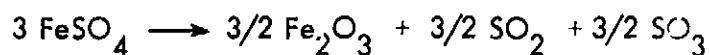
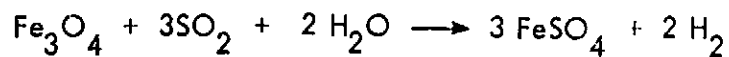
PROCESS NUMBER 12: Beulah  
General Electric  
Wenford and Hanneman



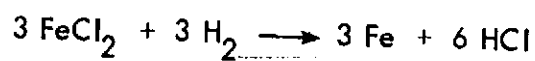
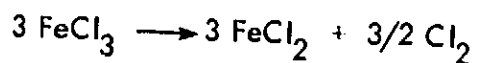
PROCESS NUMBER 13: Catherine  
General Electric  
Wenford and Hanneman



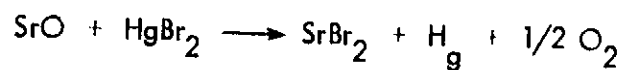
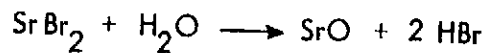
PROCESS NUMBER 14: Cycle C-5  
Institute of Gas Technology  
Pangborn and Sharer



PROCESS NUMBER 15: Cycle A-2  
Institute of Gas Technology  
Pangborn and Sharer

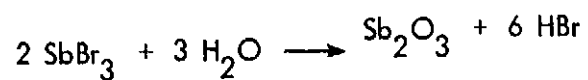
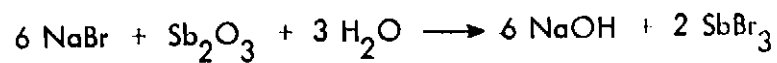
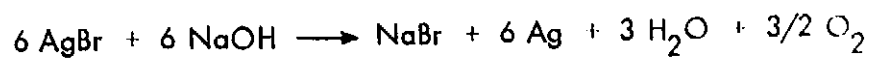
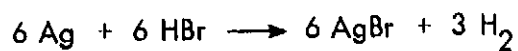


PROCESS NUMBER 16: Strontium Bromide  
Euratom  
deBeni



PROCESS NUMBER 17:

Karlsruhe Process  
Gesellschaft für Kernforschung mbH.  
Dorner and Keller



PROCESS NUMBER 18:

Sulfur Cycle  
Westinghouse Electric Corporation  
Brecher and Wu

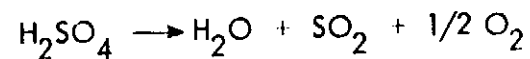
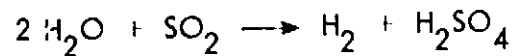


TABLE 3.4.3.  
CHEMICAL MAKE-UP COST ANALYSIS

Process Number	Chemicals	Loss Rate Kg/Day	Cash Flow \$/Day	Chemical Make-Up Cost	
				c/10 <sup>6</sup> Btu	c/GJ
1	V at \$11.02/Kg (\$5/Lb)	121,400	1,338,000		
	Cl <sub>2</sub> at \$0.088 Kg (\$80/Ton)	42,100	3,700		
	Total	163,500	1,341,700	409.00	387.00
2	Cs at \$220.46/Kg (\$100/Lb)	159,800	35,230,000		
	Total	159,800	35,230,000	10,750.00	10,180.00
3	Fe at \$0.11 (\$100/Ton)	23,400	2,570		
	C at \$0.022 (\$20/Ton)	7,300	160		
	Total	30,700	2,730	0.84	.80
4	SnO <sub>2</sub> at \$2.05/Kg (\$0.93/Lb)	90,700	186,000		
	Total	90,700	186,000	56.7	53.7
5	Cl <sub>2</sub> at \$0.088/Kg (\$80/Ton)	42,100	3,700		
	Total	42,100	3,700	1.13	1.07
6	Hg at \$11.02/Kg (\$5/Lb)	241,600	2,662,000		
	Cl <sub>2</sub> at \$0.088/Kg (\$80/Ton)	42,100	3,700		
	Total	283,700	2,665,700	813.00	770.00

TABLE 3.4.3 (CONTINUED)

Process Number	Chemicals	Loss Rate Kg/Day	Cash Flow \$/Day	Chemical Make-Up Cost	
				¢/10 <sup>6</sup> Btu	¢/GJ
7	CaO at \$0.022/Kg (\$20/Ton)	33,700	740		
	Br <sub>2</sub> at \$0.55/Kg (\$500/Ton)	96,200	53,000		
	Hg at \$11.02 (\$5/Lb)	120,800	1,331,200		
	Total	250,700	1,384,940	422.00	400.00
8	Fe at \$0.11/Kg (\$100/Ton)	46,900	5,160		
	Cl <sub>2</sub> at \$0.088/Kg (\$80/Ton)	63,100	5,550		
	Total	110,000	10,710	3.28	3.11
9	KOH at \$0.022/Kg (\$20/Ton)	67,300	1,480		
	Se at \$15.43/Kg (\$7/Lb)	47,400	731,400		
	Total	114,700	732,880	224.00	212.00
10	C at \$0.022/Kg (\$20/Ton)	7,300	160		
	As <sub>2</sub> O <sub>3</sub> at \$0.11/Kg (\$100/T)	118,900	13,100		
	Total	126,200	13,260	4.05	3.84
11	Fe at \$0.11/Kg (\$100/Ton)	46,900	5,160		
	Cl <sub>2</sub> at \$0.088/Kg (\$80/Ton)	42,100	3,700		
	MgO at \$0.094/Kg (\$85/Ton)	24,000	2,260		
Total	113,000	11,120	3.41	3.23	



TABLE 3.4.3 (CONTINUED)

Process Number	Chemicals	Loss Rate Kg/Day	S/Day	Chemical Make-Up Cost	
				¢/106 Btu	¢/GJ
12	CuCl at \$0.66/Kg (30¢/Lb)	76,900	50,800		
	Cl <sub>2</sub> at \$0.088/Kg (\$80/Ton)	42,100	3,700		
	MgO at \$0.094/Kg (\$85/Ton)	24,000	2,260		
	Total	143,000	56,760	17.3	16.4
13	LiI at \$4.41/Kg (\$2/Lb)	161,100	710,400		
	Ni at \$0.66/Kg (30¢/Lb)	35,500	23,400		
	Total	196,600	733,800	224.00	212.00
14	Fe at \$0.11/Kg (\$100/Ton)	23,400	2,570		
	S at \$0.033/Kg (\$30/Ton)	19,200	630		
	Total	42,600	3,200	0.98	.93
15	Fe at \$0.11/Kg (\$100/Ton)	46,900	5,160		
	Cl <sub>2</sub> at \$0.088/Kg (\$80/Ton)	189,300	16,660		
	Total	236,200	21,820	6.67	6.32
16	SrBr <sub>2</sub> at \$1.70/Kg (\$0.77/Lb)	197,100	335,000		
	Hg at \$11.02/Kg (\$5/Lb)	120,800	1,331,000		
	Total	317,900	1,666,000	509.00	482.00

TABLE 3.4.3 (CONTINUED)

Process Number	Chemicals	Loss Rate Kg/Day	\$/Day	Chemical Make-Up Cost	
				¢/10 <sup>6</sup> Btu	¢/GJ
17	Ag at \$141/Kg (\$64/Lb)	129,800	18,302,000		
	Br <sub>2</sub> at \$0.55/Kg (\$500/Ton)	96,200	53,000		
	Sb <sub>2</sub> O <sub>3</sub> at \$0.66/Kg (30¢/Lb)	112,900	74,500		
	NaOH at \$0.088/Kg (\$80/T)	48,100	4,200		
	Total	387,000	18,433,700	5,628.0	5,330.0
18	S at \$0.033/Kg (\$30/Ton)	19,200	630		
	Total	19,200	630	0.19	.18

TABLE 3.4.4

## SUMMARY OF PHASE I CHEMICAL MAKE-UP COST ESTIMATE

<u>Process Number</u>	<u>Cycle Name</u>	<u>Make-Up Chemical Cost</u>	
		<u>¢/GJ</u>	<u>¢/10<sup>6</sup> Btu</u>
18	Westinghouse Sulfur Cycle	0.18	0.19
3	IGT Steam-Iron-Carbon Dioxide	0.80	0.84
14	IGT Cycle C-5	0.93	0.98
5	Air Products - HCl Electrolysis	1.07	1.13
8	Euratom Mark-9	3.11	3.28
11	General Electric - Agnes	3.23	3.41
10	L. Livermore Lab - Methane - Methanol	3.84	4.05
15	IGT Cycle A-2	6.32	6.67
12	General Electric - Beulah	16.40	17.30
4	Gaz de France Tin Oxide Process	53.70	56.70
13	General Electric - Catherine	212.00	224.00
9	Lawrence L. Lab - Selenium Cycle	212.00	224.00
1	General Motors Vanadium Chloride	387.00	409.00
7	Euratom Mark-1	400.00	422.00
16	Euratom Strontium Bromide	482.00	509.00
6	IGT Mercury Chloride Electrolysis	770.00	813.00
17	Karlsruhe Process	5,330.00	5,628.00
2	Cesium Oxide Process	10,180.00	10,750.00

Only after a cycle has been shown to possess low make-up costs was its feasibility and efficiency examined in detail. The second phase of evaluation is concerned with verifying that the proposed reactions will proceed as written, as well as ascertaining that the cycle truly offers the potential of competing with other hydrogen production methods. Eight processes, summarized in Table 3.4.5 were considered.

Process No. 3, the IGT Steam-Iron-Carbon Dioxide Cycle was eliminated as it contained a reaction that was more difficult to conduct than the direct decomposition of water. This can be seen by rewriting the process as follows:

Water Vaporization	$\frac{\Delta G^\circ}{298}$	$\frac{\Delta H^\circ}{298}$	$\frac{T\Delta S^\circ}{298}$
(1) $H_2O_{(l)} \rightarrow H_2O_{(g)}$	8.51 KJ	44.02 KJ	35.5 KJ
Shift Conversion			
(2) $CO_{(g)} + H_2O_{(g)} \rightarrow$	-28.56 KJ	-41.17 KJ	-12.61 KJ
Carbon Dioxide Reduction			
(3) $CO_{2(g)} \rightarrow CO_{(g)} + 1/2 O_{2(g)}$	257.2 KJ	283.0 KJ	25.75 KJ

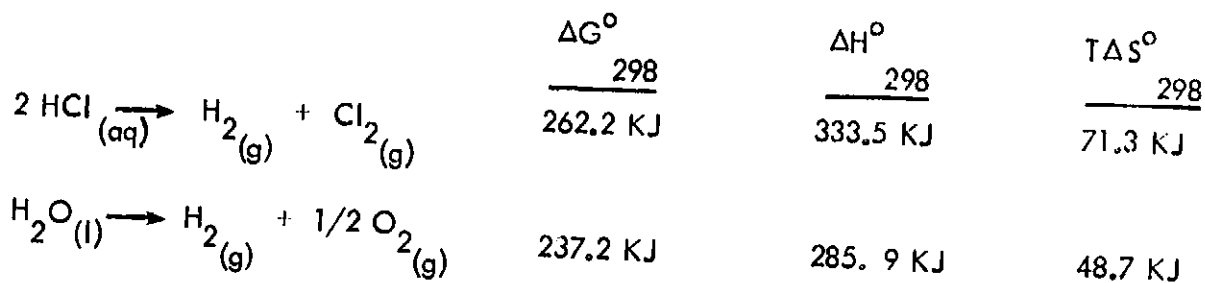
Reactions (1) and (2) are conventional. Reaction (3), if conducted mechanically, requires more mechanical work than electrolysis (257.2 KJ compared to 237.2 KJ). If the reaction is conducted thermally, temperature and energy inputs comparable to those required to decompose water directly are necessary.

Not only will considerable ingenuity be required in conducting Reaction 3, but a well-conceived separation system will also be required for the CO/O<sub>2</sub> mixture. The oxidation of carbon monoxide to the dioxide can occur rapidly, even in the absence of catalysts. As a result, a potentially serious and perhaps explosive reaction reversal can occur.

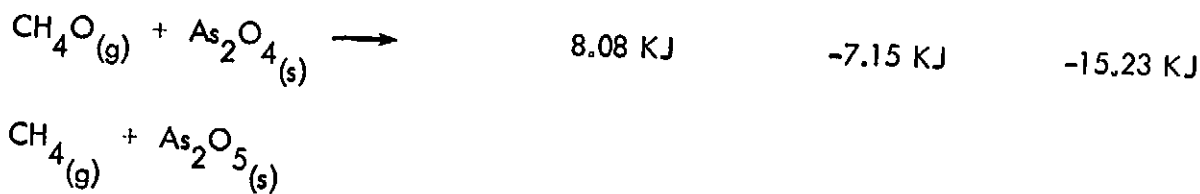
Process No. 5, the Air Products - HCl Electrolysis cycle was discarded as the electrolysis of HCl requires more power per unit of hydrogen production than direct water electrolysis. This can be seen by the following comparison:

TABLE 3.4.5  
PROCESSES CONSIDERED FOR PHASE II EVALUATION - REACTION FEASIBILITY

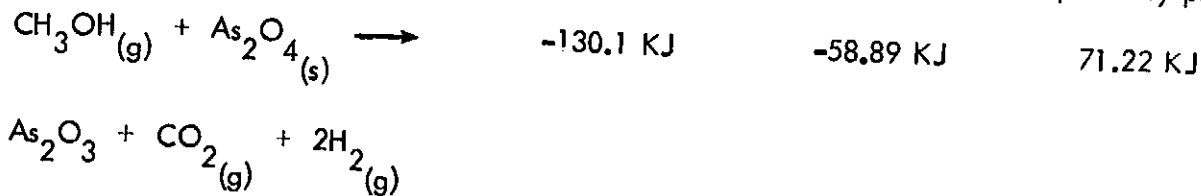
<u>Process Number</u>	<u>Cycle Name</u>
3	IGT Steam-Iron Carbon Dioxide
5	Air Products - HCl Electrolysis
8	Euratom Mark-9
10	Lawrence Livermore Lab - Methane - Methanol
11	General Electric - Agnes
14	IGT Cycle C-5
15	IGT Cycle A-2
18	Westinghouse Sulfur Cycle



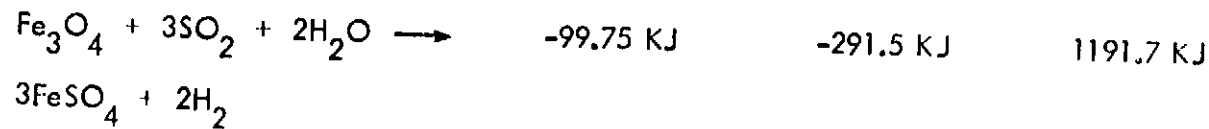
Process No. 10, the Lawrence Livermore Laboratory Methane-Methanol cycle was eliminated because it contained a reaction unfavorable with respect to competing reactions. Methanol is an alcohol, not an oxide. Its reduction to methane is not to be expected. The reaction



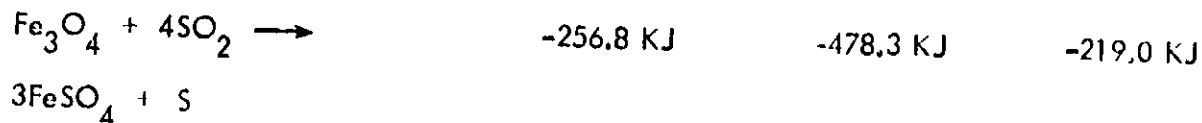
may proceed; however, passing hot methanol over heated arsenic oxides will probably produce:



Process No. 14, the IGT cycle C-5, was also eliminated because its first reaction is not expected to proceed. The reaction is written as:



A thermodynamically more favorable reaction is:



As a result of this phase of the evaluation, only the four cycles listed in Table 3.4.6 appear sufficiently attractive to warrant an investigation of the process thermodynamics.

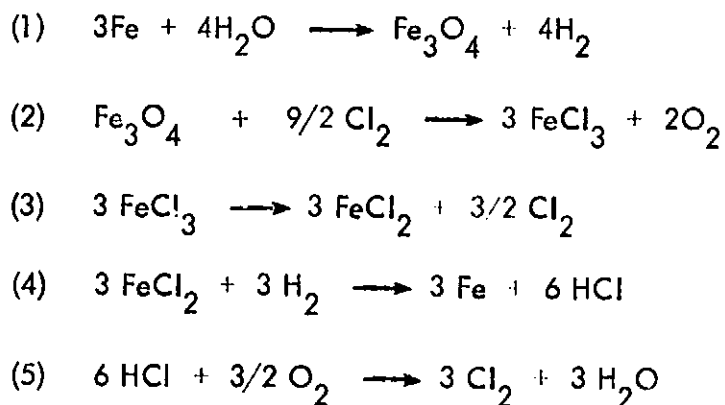
TABLE 3.4.6

## PROCESSES CONSIDERED FOR THERMODYNAMIC EVALUATION

<u>Process Number</u>	<u>Cycle Name</u>
8	Euratom Mark-9
11	General Electric - Agnes
15	IGT Cycle A-2
18	Westinghouse Sulfur Cycle

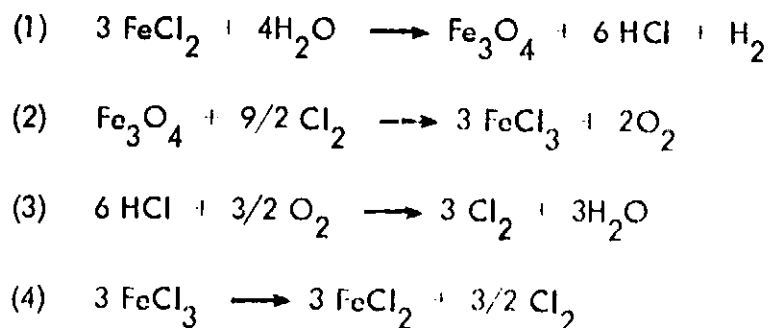
In order to ensure a more realistic evaluation of the potential process efficiencies, Process No. 15, the IGT Cycle A-2, was modified.

The cycle as originally proposed was:



As written, this cycle is inefficient due to the decomposition of four moles of water in Reaction (1) followed by the subsequent recombination of three of these in Reactions (4) and (5). A more efficient cycle is obtained by combining Reactions (1) and (4). This is now:

IGT Cycle A-2 (Modified)



Examination of the four remaining cycles shows only two to be independent. Note that the General Electric Agnes process, the Euratom Mark-9, and the modified IGT Cycle A-2 are all nearly the same. Each begins by hydrolyzing ferrous chloride to produce hydrogen. Each thermally reduces ferric chloride to provide chlorine. The processes differ only in the manner in which  $\text{Fe}_3\text{O}_4$  is converted to  $\text{FeCl}_3$ . The similarities in these cycles are shown in Figure 3.4.1. All of these cycles appear technically feasible.

A first estimate of the thermal efficiency of each of the four cycles may be obtained by examining the thermodynamics of the reactions in the cycle. A reversible process occurring at constant temperature and pressure requires a work input equal to  $\Delta G$  and a heat input equal to  $T\Delta S$ . Since  $\Delta G = \Delta H - T\Delta S$ , one has that  $Q = W = \Delta H$ . Varying the temperature changes the ratio of heat to work required by the reaction.  $T\Delta S_{298}^\circ$ , however, represents the minimum amount of heat the reaction must reject to sink at 298K. This heat rejection occurs regardless of the temperature of the heat source during the process. Since 285.9 KJ of process energy are required to decompose water, the minimum amount of heat to drive the decomposition cycle

$$\text{is } Q_{\min} = 285.9 - \sum_i (T\Delta S_{298}^\circ)_i,$$

$$\text{where } (T\Delta S_{298}^\circ)_i < 0.$$

This correspondingly defines the maximum thermal efficiency as

$$E_{\max} = \left( \frac{285.9}{Q_{\min}} \right) \times 100\%.$$

Using a 1200K heat source, a second estimate of the process thermal efficiency can be provided. Assuming ideal recuperative heat exchange, Carnot efficiencies in all power cycles, and ideal works of separation yields the results shown under the limiting thermal efficiency column in Table 3.4.7.

As Table 3.4.7 shows, when compared with other published cycles, the Westinghouse Sulfur Cycle offers the potential for the lowest cost hydrogen. The make-up chemical cost is lower, the thermal efficiency is higher, and the process can benefit more from the development of even higher heat source temperatures. A number of additional considerations are summarized in Table 3.4.8 and these deserve comment.

The Westinghouse Sulfur Cycle was invented to operate energized with a gas cooled nuclear reactor and supplying its hydrogen and oxygen outputs to a coal process. As a result, it possesses interfaces compatible to both systems. This results in several very desirable additional features beyond its low chemical cost and high efficiency.



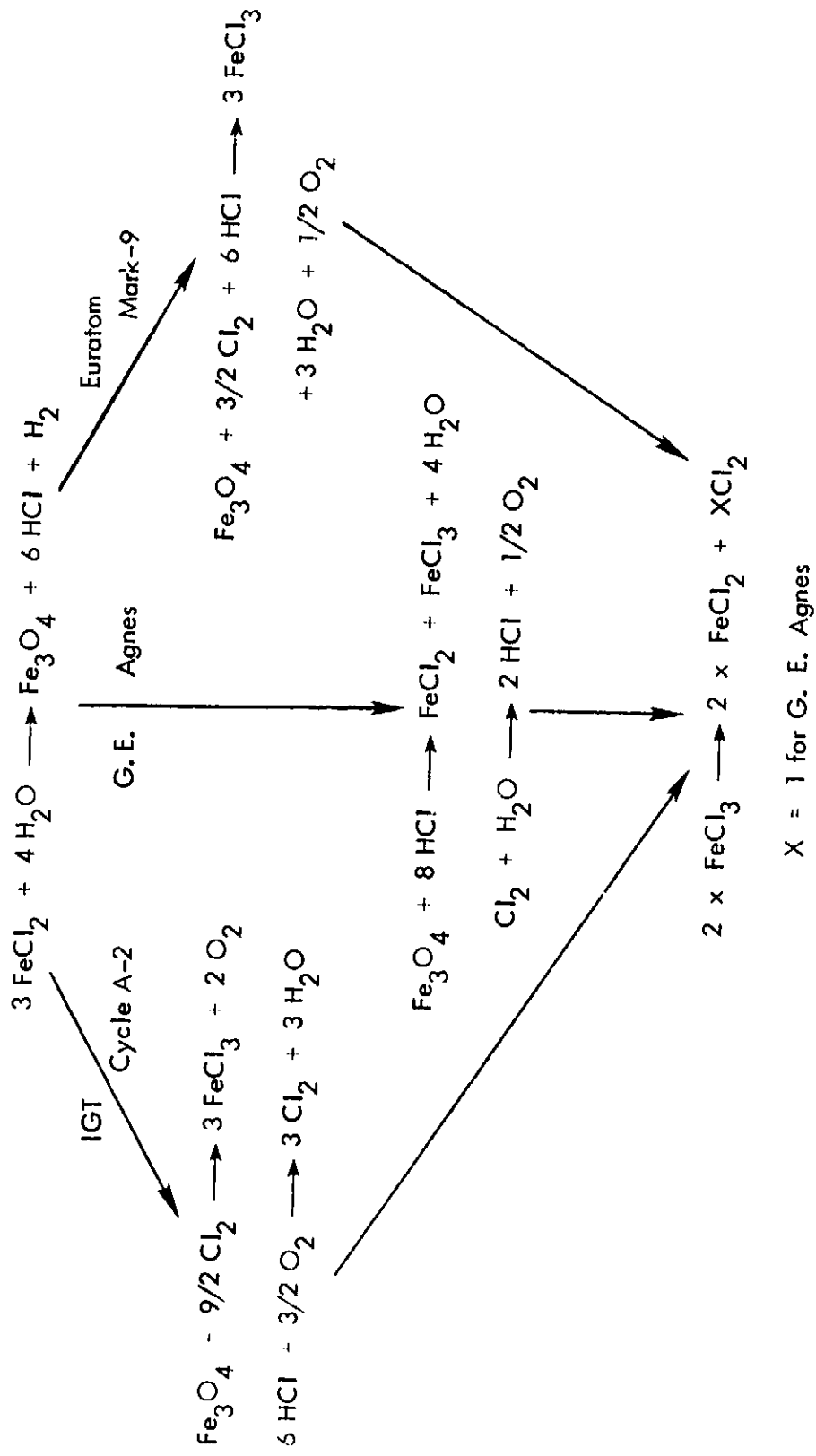


Figure 3.4.1 Comparison of Euratom, G.E., and I.G.T. Iron and Chlorine Cycles

TABLE 3.4.7

RESULTS OF PROCESS SELECTION

Process Number	Process Identification	Make-Up Chemical Cost, ¢/GJ	Reaction Feasibility		Maximum Thermal Efficiency	Limiting Thermal Efficiency
			Yes	No		
18	Westinghouse Sulfur Cycle	0.18	X		90.52%	78.0
3	IGT-Stream-Iron-Carbon Dioxide	0.80		X		
14	IGT Cycle C-5	0.93		X		
5	Air Products-HCl Electrolysis	1.07		X		
8	Euratom Mark-9	3.11	X		65.51%	58.3
11	General Electric-Agnes	3.23	X		67.56%	
10	LLL-Methane-Methanol	3.84		X		
15	IGT Cycle A-2	6.32	X		65.51%	
12	General Electric-Boulah	16.40				
4	Gasde France-Tin Oxide	53.70				
13	General Electric-Catherine	212.00				
9	LLL-Selenium Cycle	212.00				
1	General Motors - Vanadium Chloride	387.00				
7	Euratom Mark-1	400.00				
16	Euratom-Sr-Strontium Bromide	482.00				
6	IGT-Mercury Chloride	770.00				
17	Karlshruhe Process	5,330.00				
2	Cesium Oxide	10,180.00				

At no point in the process does the nuclear heat source provide thermal energy to a reducing gas. Reducing gases, due to high hydrogen partial pressures, can lead to hydrogen accumulation within the coolant of the nuclear heat transport system. This would result in the reaction of the hydrogen with the graphite nuclear core materials and its attendant structural weakening.

The Sulfur Cycle can be operated to provide hydrogen at pressure thereby reducing the cost of gas compression equipment. The electrolyzer, if designed to maintain a differential pressure between the anode and cathode, cannot only provide pressurized hydrogen, but lower its power input requirements as well.

All thermochemical water decomposition processes, if directly heated, can operate on any convenient thermal source. The Westinghouse process can be fueled with gas, oil, or coal. As a recent Chemical and Engineering News article confirms (Reference 31), the  $SO_3$  reduction can be accomplished in a solar collector. Thus the process, if necessary or economical, can be solar powered.

Last, but not least, is the consideration that impurities in the hydrogen and oxygen supplied to the ultimate use process do not jeopardize operation of that system. Industrial processes and equipment have not generally been designed in expectation of large quantities of halides, vanadium, cesium, tin, mercury, arsenic, copper, silver, strontium, or antimony compounds in their feedstocks. They have been, however, designed for operation with sulfur containing feedstocks. As a result, the purity of hydrogen and oxygen from a sulfur-based water decomposition process can be adjusted to provide the best overall system economics containing feedstocks. As a result, the purity of hydrogen and oxygen from a sulfur-based water decomposition process can be adjusted to provide the best overall system economics.

TABLE 3.4.8

FINAL PROCESS SUMMARY

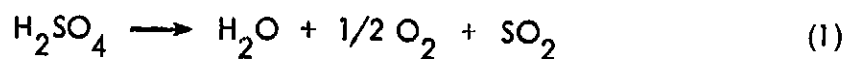
<u>Item</u>	<u>Euratom Mark 9</u>	<u>Westinghouse Sulfur</u>
Cost of Make-Up Chemicals, ¢/GJ	3.11	0.18
Maximum Achievable Efficiency	65.51%	90.52%
Thermodynamic Efficiency	58.3 %	78.0 %
Capable of Solar Powering	No	Yes
Impurities to User Process	Halides	Sulfur

### 3.4.3 Westinghouse Water Decomposition Process

The Westinghouse hydrogen production process is a two-step thermochemical cycle for decomposing water into hydrogen and oxygen. Oxides of sulfur serve as recycling intermediates within the process. The use of sulfur compounds results in several process advantages:

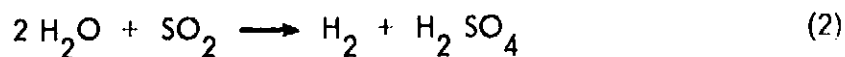
- Sulfur is abundant, inexpensive, and substantially non-toxic.
- An assured supply of make-up sulfur is available from coal conversion and stack gas scrubbing processes.
- Sulfur is an item of commerce and processes, equipment, catalysts, literature, and distribution systems for it and its compounds abound.
- Sulfur assumes a variety of valence states, thereby facilitating its use in oxidation-reduction reactions.
- The properties of sulfur and its compounds are well documented, thereby reducing the amount of basic information needed in a process development effort.
- Environmental regulations for the use of sulfur exist today, reducing uncertainties in the design of process equipment.

The process, in its most general form, consists only of two chemical reactions - one for producing oxygen and the other for producing hydrogen. The production of oxygen occurs via the thermal reduction of sulfur trioxide obtained from sulfuric acid.

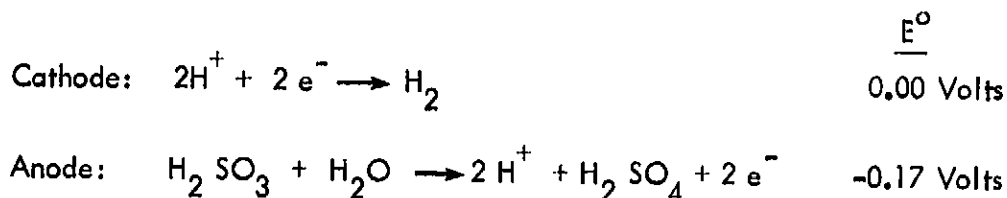


The equilibrium for Reaction 1 lies to the right at temperatures above 1000K. Catalysts are available for accelerating the rate of sulfur trioxide reduction to sulfur dioxide and oxygen. The results of Westinghouse's evaluation of two of these catalysts is reported elsewhere in this document.

The process is completed by using the sulfur dioxide from the thermal reduction step to depolarize the anode of a water electrolyzer. The overall reaction occurring electrochemically is



This is comprised of the individual reactions



As is apparent by summing Reactions 1 and 2, the overall process decomposes water into hydrogen and oxygen and involves only sulfur oxides as recycling intermediates. Although electrical power is required in the electrolyzer, much smaller quantities than those necessary in conventional electrolysis are needed. The theoretical voltage to decompose water is 1.23 V, with many commercial electrolyzers requiring over 2.0 V. The power requirements for Reaction 2 (0.17 volts at unit activity for reactants and products) are thus seen to be less than 15 percent of those required in conventional electrolysis. This changes dramatically the theoretical heat and work required to decompose water and leads to high thermal efficiencies.

The process is shown schematically in Figure 3.4.2. Hydrogen is generated electrolytically in an electrolysis cell which anodically oxidizes sulfurous acid to sulfuric acid while simultaneously generating hydrogen at the cathode. Sulfuric acid formed in the electrolyzer is sent to a surge tank from where it is fed to two vaporizers in series. The first of these is a recuperative heat exchanger heated by the effluent from the high temperature sulfur trioxide reduction reactor. The second is heated by helium from the VHTR. The sulfur trioxide - steam mixture from the second vaporizer flows to the helium heated reduction reactor where sulfur dioxide and oxygen are formed. These gases are subsequently cooled against the incoming acid and unreacted sulfur trioxide is recovered as sulfuric acid in a knock-out system. Wet sulfur dioxide and oxygen flow to the separation system. Steam is first condensed, following which the  $\text{SO}_2/\text{O}_2$  mixture is compressed and sulfur dioxide recovery effected.

Bulk sulfur dioxide removal is accomplished by condensation against cooling water. Final removal is achieved by condensation against low-temperature oxygen. This refrigeration and some auxiliary power production is generated by expansion of the oxygen stream prior to its venting.

Two important trade-offs exist in specifying process conditions for the flowsheet shown. The first relates to the concentration of the sulfuric acid leaving the electrolyzer. Operation at very high acid concentrations raises the power requirements in the electrolyzer while simultaneously reducing the mass rates and thermal energy demand in the acid vaporization, decomposition, and recovery loop. Similarly, operation at very low acid concentrations lowers the electrolyzer power requirements, but leads to high mass rates and thermal demands in the acid decomposition loop. An optimal acid concentration exists.

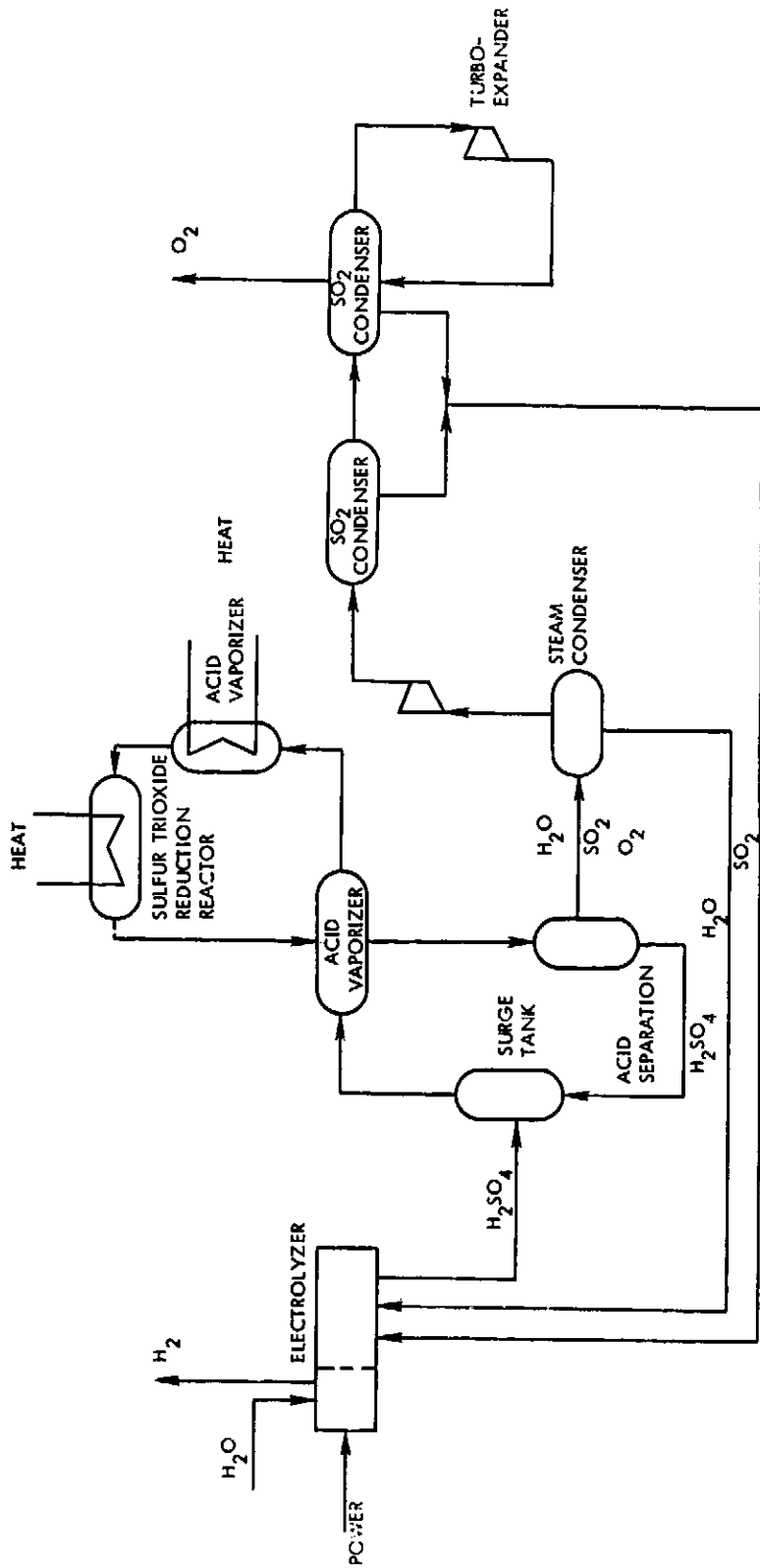


Figure 3.4.2 Sulfur Cycle Schematic Flowsheet

Pressure is important due to the pressurized  $\text{SO}_2/\text{O}_2$  recovery system employed in the process as well as the pressure dependence of the sulfur trioxide reduction reaction (the equilibrium conversion at a given temperature declines with increasing system pressure). Operation at low pressures leads to high conversions, low recycle rates, and large compression requirements. Operation at higher pressures reduces the compressor duties, but at the expense of the sulfuric acid recycle rate. Thus, an optimal pressure similarly exists.

Both the optimum acid concentration and the optimum pressure vary with the heat source temperature. Similarly, overall thermal efficiency rises with increasing heat source temperature. Raising the heat source temperature increases power cycle efficiencies and shifts the optimal acid concentration to more concentrated solutions. This in turn reduces the thermal requirements in the acid decomposition system. Similarly, higher heat source temperatures enable higher system pressures to be employed without sacrificing the conversion per pass achieved in the sulfur trioxide reduction reactor. This reduces compression requirements and improves the process efficiency.

For the purpose of the comparative evaluation of hydrogen generation systems performed, the water decomposition system was considered to have the process flowsheet presented schematically in Figure 3.4.2 and in more detail in Section 4.5. The principal operating and performance characteristics of the process are given in Table 3.4.9. These characteristics will, as a result of the work done in Task II of this contract, be modified for the Task III conceptual design to be reported upon in a separate volume.

The process, as currently defined, is arranged for its primary energy inputs to be made as electricity in the electrolyzer and heat, from the intermediate heat transport loop of the nuclear heat source, to the acid vaporizer and the  $\text{SO}_3$  reduction reactor. Other heat sources, including combustion, solar, or geothermal, can provide the heat energy for the  $\text{SO}_3$  reduction reactor and the generation of electric power.

This alternate fueling capability provides the flexibility to consider operation of the hydrogen production facility with any economic source of heat and electric power. Alternate energy sources for the water decomposition process are discussed in more detail in Section 3.4.4.

TABLE 3.4.9

PRINCIPAL OPERATING AND PERFORMANCE CHARACTERISTICS OF THE  
WESTINGHOUSE SULFUR CYCLE WATER DECOMPOSITION SYSTEM

General

Hydrogen Production Rate	$10.09 \times 10^6$ standard m <sup>3</sup> /day	( $379 \times 10^6$ SCFD)
Hydrogen Purity	99.9 volume percent	
Oxygen Production Rate	305,500 kg/hr	(673,000 lb/hr)
Nuclear Heat Source Rating	3220 MWt	
Net Process Thermal Efficiency	47 percent	

Electrolysis

Acid Concentration	80 wt percent	
Pressure	2586 kPa	(375 psia)
Temperature	361 K	(190°F)
Electrolyzer Power Req't	482 Mwe	
Cell Voltage, Nominal	0.48 volts	
Cell Current Density, Nominal	2000 A/m <sup>2</sup>	(186 A/ft <sup>2</sup> )

Sulfur Trioxide Reduction System

Peak Temperature	1144 K	(1600°F)
Operating Pressure	2068 kPa	(300 psia)

Sulfur Dioxide - Oxygen Separator System

SO <sub>2</sub> Liquefaction Pressure	5171 kPa	(750 psia)
Oxygen Discharge Pressure	517 kPa	( 75 psia)



#### 3.4.4 Energy Sources for the Westinghouse Sulfur Cycle

The Sulfur Cycle water decomposition process, in its reference configuration, has its primary energy inputs made as electricity in the electrolyzer and heat, from the intermediate heat transport loop of a nuclear heat source, to the  $\text{SO}_3$  reduction reactor and the acid vaporizer. This is the process arrangement described in Section 3.4.3 and illustrated in Figure 3.4.2. Other heat sources, including fossil fuel combustion, solar, or geothermal, can provide the thermal energy for the process steps and the generation of electric power. The thermal energy would be introduced into the process in a manner dependent upon the characteristic of the heat source. The electric energy needed for the electrolyzers would be produced in the manner most appropriate for each of the alternate fuels.

For the process flowsheet used in the comparative evaluation, heat from alternate energy sources could be introduced to the process in the same manner as for the nuclear powered system. The process heat exchanger ( $\text{SO}_3$  reduction reactor) and acid vaporizer design could, for example, be modified for heat inputs from an intermediate fluid which in turn is heated by the energy source. Alternately, the process heat exchanger and acid vaporizer could be designed for direct "firing", much like conventional reformers or boilers. The specific approach to be used would depend upon design optimization for each of the potential energy sources.

Other process variations of the Westinghouse Sulfur Cycle can be developed which can utilize any convenient or economical source of process energy. One such process alternate that has been investigated can accept the process energy either directly as a fuel gas or indirectly as thermal energy entering the system through a heat exchanger. This process alternative uses a different acid concentration system and a different approach to the sulfur trioxide reduction than the reference process.

When the alternate process configuration is operating in the directly fueled mode, any gaseous fuel may be employed. This includes not only light hydrocarbon gases, but also the product gases obtained from air-blown coal or oil gasifiers, as well as any process or plant fuel gases which may be available. The sulfur content of the feed gas is unimportant as the hydrogen process contains provisions for sulfur removal. No oxygen plants or acid gas removal facilities are required and the hydrogen purity is independent of the feed gas composition.

When operated in the indirectly fueled mode, with the indirect addition of thermal energy, oxygen as well as hydrogen production is achieved. Under these circumstances, fuel or flue gas desulfurization may be necessary to meet environmental regulations (as it would be if the gas were to be burned elsewhere), but, as before, low Btu fuels can be employed without affecting either the hydrogen or oxygen purities.

The two operating modes of the process are illustrated in Figures 3.4.3 and 3.4.4. As in the reference configuration, hydrogen is generated electrolytically in an electrolysis cell which anodically oxidizes sulfurous acid to sulfuric acid while simultaneously generating hydrogen at the cathode.

The regeneration of  $\text{SO}_2$  from the electrolyzer sulfuric acid effluent is accomplished by chemically extracting, as ferric sulfate, the sulfur trioxide formed in the electrolyzer, followed by the subsequent thermal decomposition of the sulfate into iron oxide, oxygen, and  $\text{SO}_2$ . The extraction of the sulfur trioxide takes place in two stages as shown in Figure 3.4.3. The electrolyzer effluent is assumed to contain about 40 W/O  $\text{H}_2\text{SO}_4$  (Point B). Iron oxide is dissolved into this to the limits of its solubility at 333K (Point C). This solution, when heated to 473K produces a liquid phase containing about 15 W/O  $\text{H}_2\text{SO}_4$  (Point A). This solution is cooled and recycled to the electrolyzer where its concentration is once again increased by the reactions given earlier to 40 W/O  $\text{H}_2\text{SO}_4$ . Leaving the crystallizer is a hydrated ferric sulfate having the composition  $\text{Fe}_2\text{O}_3 \cdot 2\text{SO}_3 \cdot \text{H}_2\text{O}$  and consisting of a mixture of  $\text{Fe}_2\text{O}_3 \cdot 3\text{SO}_3$  and  $\text{Fe}_2\text{O}_3 \cdot 3\text{H}_2\text{O}$ . Steam requirements in the crystallizer are met by evaporating boiler feed water injected into the oxide coolers contained in the dryer and decomposition reactors.

The mixture of  $\text{Fe}_2\text{O}_3 \cdot 3\text{SO}_3$  and  $\text{Fe}_2\text{O}_3$  obtained from the crystallizer yields, after decomposition,  $\text{SO}_3/\text{H}_2\text{O}$  ratios comparable to those obtained in fuming sulfuric acid. This concentration is achieved from a 40 percent feed acid without evaporating large quantities of water as is required in thermal concentrators. The inclusion of this system into the process enables the electrolyzer to operate with low activities of sulfuric acid, thereby with low power requirements, while simultaneously avoiding the need to recycle large quantities of water into the  $\text{SO}_3$  reduction system. The need to employ a thermal concentrator with the subsequent generation of large quantities of low pressure steam is similarly avoided. The use of ferric sulfate within the process offers additional advantages which become apparent in examining the operation of the sulfate decomposition system. The hydrated ferric sulfate leaving the crystallizer is fed next into a dryer-classifier and then into a decomposition reactor. These vessels are fluidized beds operating at pressures between 2000 and 5000 kPa (20 to 50 atm). Both contain three stages. The upper portion of the bed is an expanded section for lighter  $\text{Fe}_2\text{O}_3$  particles, the central section is narrower and contains  $\text{Fe}_2\text{O}_3 \cdot 3\text{SO}_3$  and  $\text{Fe}_2\text{O}_3$ , while the bottom section is the oxide cooler which accepts overflow from the upper section of each bed.

Considering first the system operation with low Btu gas, the hydrated ferric sulfate is fed through lock hoppers and into the central section of the dryer-classifier. Combustion of low-Btu gas provides the thermal energy necessary to decompose  $\text{Fe}_2\text{O}_3 \cdot 3\text{H}_2\text{O}$  into iron oxide and steam. The lighter  $\text{Fe}_2\text{O}_3$ , after decomposition, is blown into the upper section of the bed. Overall temperature is maintained above that required to decompose  $\text{Fe}_2\text{O}_3 \cdot 3\text{H}_2\text{O}$  but below that at which  $\text{Fe}_2\text{O}_3 \cdot 3\text{SO}_3$  decomposes. In spite of this, local hot spots near the distributor will liberate some  $\text{SO}_3$  which will be recaptured in the upper bed section. Iron

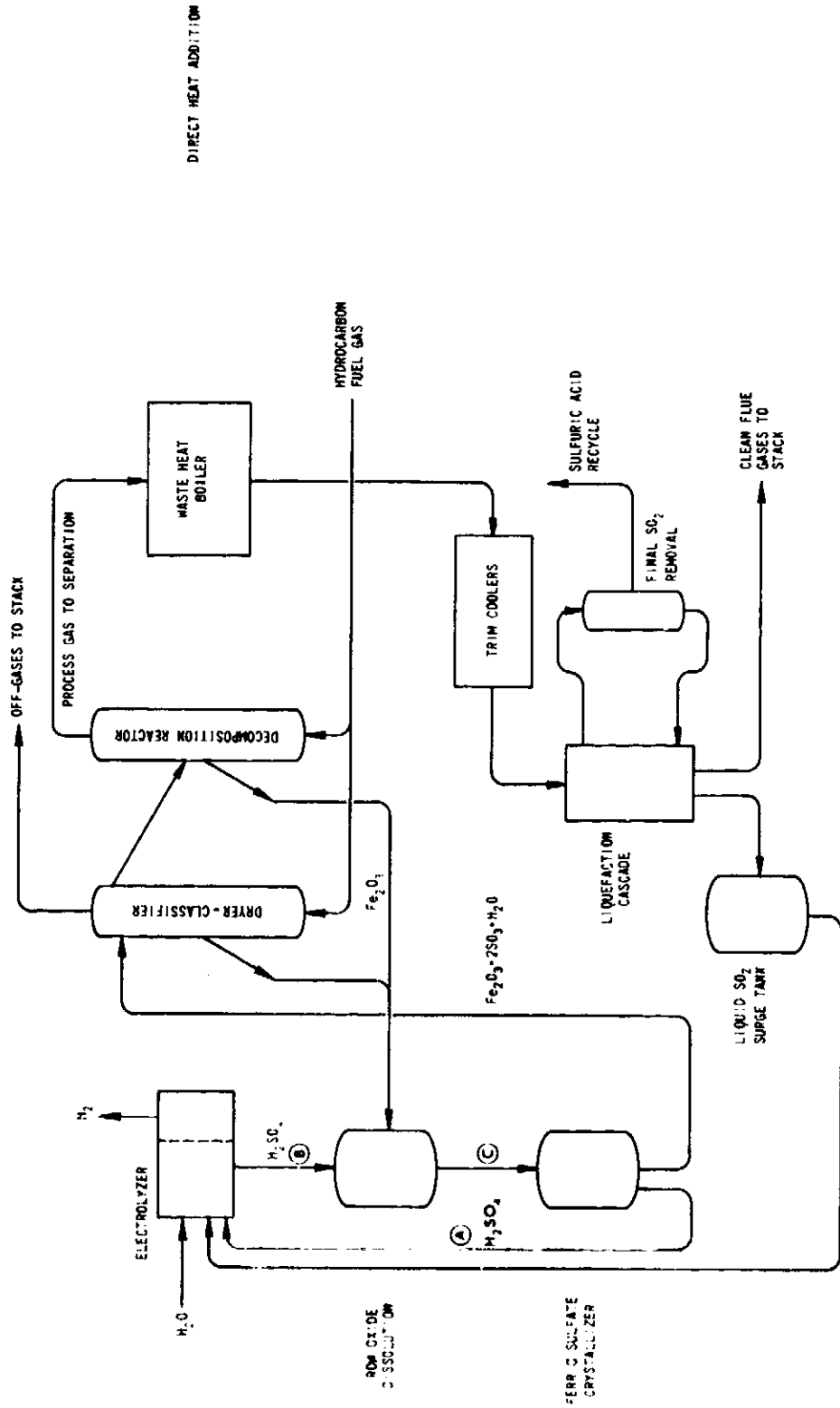


Figure 3.4.3 Direct Heat Mode of Operation for the Westinghouse Hydrogen Production System

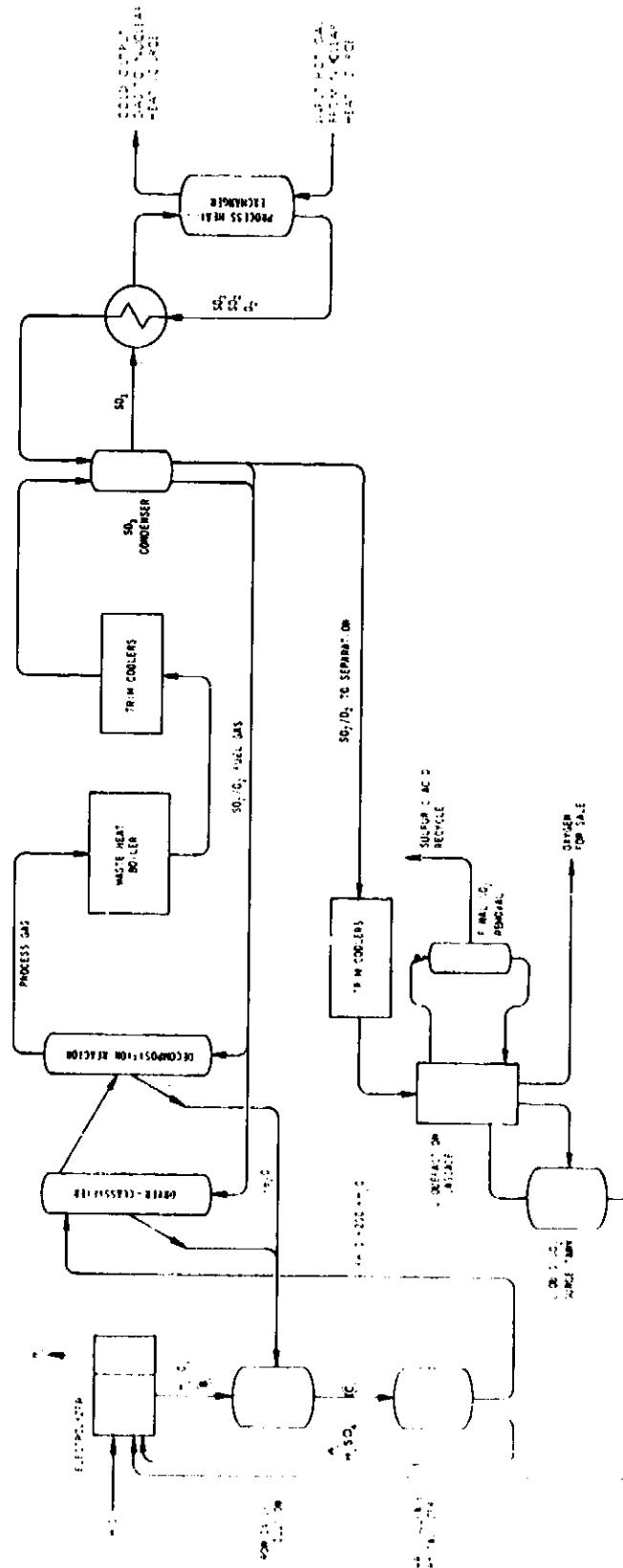
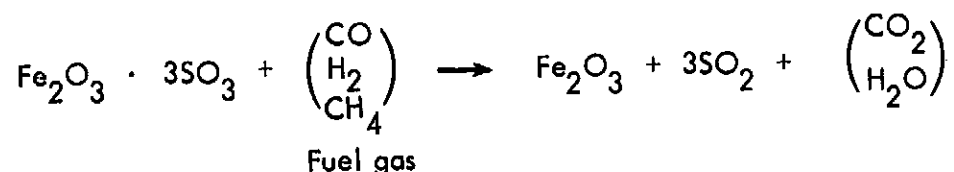


Figure 3.4.4 Indirect Heat Mode of Operation for the Westinghouse Hydrogen Production System

oxide overflow from the upper section flows to the cooler. This portion of the vessel is fluidized with steam and contains nozzles for injecting boiler feed water into the bed. The cooling of the  $\text{Fe}_2\text{O}_3$  prior to letdown is accomplished while generating process steam for use in the crystallizer. Ferric sulfate contained in the central section of the bed flows to the decomposition reactor.

The decomposition reactor operates at the same nominal pressure as the dryer, but at higher temperatures. The fact that the bed contains  $\text{Fe}_2\text{O}_3$  - a contact catalyst for sulfuric acid manufacture - aids in establishing the equilibrium  $\text{SO}_3 \rightarrow \text{SO}_2 + 1/2 \text{O}_2$ . The oxygen liberated by the  $\text{SO}_3$  thermal reduction as well as that present in excess air added to the system serves to combust the fuel gas and to thereby provide the thermal energy necessary to decompose the ferric sulfate. Overall the following reaction occurs:

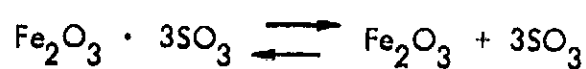


Precise air and fuel requirements in the decomposition reactor will depend upon the fuel gas employed.  $\text{SO}_2$  concentrations in excess of 20 percent are obtained with most common fuel gases. Representative outlet compositions corresponding to a low-Btu fuel gas are shown in Table 3.4.9. In this instance 8.65 moles of fuel gas and 1.312 moles of air are required to decompose one mole of  $\text{Fe}_2\text{O}_3 \cdot 3\text{SO}_3$ . The effluent from the decomposition reactor passes through a waste heat boiler which raises steam to drive the turbine generators which power the electrolyzer. The process gases are subsequently cooled and the water vapor condensed, and are then dried before entering the  $\text{SO}_2$  liquefaction cascade.

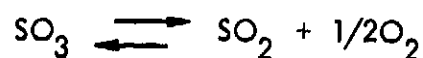
The  $\text{SO}_2$  liquefaction cascade starts with a higher temperature bulk  $\text{SO}_2$  removal step at 266K (20°F) or above, depending upon process pressure. Final  $\text{SO}_2$  removal is obtained using refrigeration generated by the process gases as they are expanded to 101 kPa (one atmosphere). Before the final gas expansion to atmospheric pressure, the remaining  $\text{SO}_2$  is removed by oxidation to  $\text{SO}_3$  and scrubbing. The resultant sulfuric acid is recycled to the iron oxidation dissolution stage or is available for sale.

In the indirectly - heated operating mode, Figure 3.4.4, the energy required for the drying and thermal decomposition of ferric sulfate is obtained by the catalytic oxidation of  $\text{SO}_2$  to  $\text{SO}_3$  within the process vessel. In the dryer, which operates at lower temperatures and elevated pressures,  $\text{SO}_3$  formation and subsequent reaction with  $\text{Fe}_2\text{O}_3$  is favored and provides the exothermic reaction heat necessary to decompose  $\text{Fe}_2\text{O}_3 \cdot 3\text{H}_2\text{O}$ .

In the sulfate decomposition reactor, two equilibria over the catalyst  $\text{Fe}_2\text{O}_3$  are established.



$$K_1 = P_{\text{SO}_3}^3$$



$$K_2 = \frac{P_{\text{SO}_2}}{P_{\text{SO}_3}} P_{\text{O}_2}^{1/2}$$

The proper operating pressure for the vessel as well as the  $\text{SO}_2/\text{O}_2$  recycle required for the decomposition energy will depend upon the system operating temperature. For process temperatures between 1200 and 1300 K, operating pressures above 4050 kPa (40 atm) can be employed (See Table 3.4.10). The effluent from the decomposition reactor contains about 31 percent  $\text{SO}_3$ , 46 percent  $\text{SO}_2$ , and 23 percent  $\text{O}_2$  for all operating temperatures and pressures shown.

The gases leaving the decomposition reactor may be cooled either by recuperative heat exchange with the incoming  $\text{SO}_2/\text{O}_2$  mixture or, as shown, by passage through a waste heat boiler prior to condensation of the sulfur trioxide. The sulfur dioxide and oxygen in the mixture are recycled to the decomposition reactor while the sulfur trioxide is vaporized and sent to the  $\text{SO}_3$  thermal reduction reactor. This reactor contains both high and low temperature contact catalysts and is indirectly heated by whatever energy source is driving the process.

The process energy required to regenerate  $\text{SO}_2$  from the sulfur trioxide formed in the electrolyzer is input here, as well as that which was input to the dryer and the ferric sulfate decomposition reactors as a result of the  $\text{SO}_2$  oxidation which occurred in those vessels. An alternate process variation would be to reduce the duty of the  $\text{SO}_3$  thermal reduction reactor by adding indirect heat to the dryer and the ferric sulfate decomposition reactor.

To do this would require heat exchange surface in a high temperature (>1144K) environment and would substantially increase the size and complexity of both the dryer and the ferric sulfate decomposition reactor. This not only complicates the operation of the system when indirectly heated, but in addition renders more difficult the use of hydrocarbon or low-Btu fuel gases within the process if oxygen recovery is not desired. Finally, the energy demands of these vessels is for process energy above, say 1144K (1600°F), which if provided in an indirectly heated fashion makes available a high temperature gas stream whose effective utilization elsewhere may be difficult.

TABLE 3.4.9  
 REPRESENTATIVE DECOMPOSITION REACTOR EFFLUENT  
 WHEN OPERATING ON LOW-BTU FUEL GAS

<u>Fuel Gas Composition</u>		<u>Decomposition Reactor Effluent</u>	
<u>Component</u>	<u>Volume %</u>	<u>Component</u>	<u>Volume %</u>
N <sub>2</sub>	54.5	N <sub>2</sub>	43.7
CO	18.6	SO <sub>2</sub>	22.7
H <sub>2</sub>	12.1	CO <sub>2</sub>	18.7
CH <sub>4</sub>	2.4	H <sub>2</sub> O	14.7
CO <sub>2</sub>	6.9	O <sub>2</sub>	0.2
H <sub>2</sub> O	5.5		
TOTAL	100.0	TOTAL	100.0

TABLE 3.4.10  
 OPERATING PRESSURE OF THE SULFATE DECOMPOSITION  
 REACTOR AS A FUNCTION OF REACTOR TEMPERATURE

<u>Temperature</u>		<u>Pressure</u>	
<u>K</u>	<u>°F</u>	<u>kPa</u>	<u>atm</u>
1000	1340	91.5	0.903
1100	1520	730.0	7.200
1200	1700	3,962.0	39.100
1300	1880	16,620.0	164.000

In evaluating these requirements, it is felt that the vessel energy demand is best met by conducting an exothermic reaction within the unit. This then enables fuel gases to be used directly if oxygen is not desired, while enabling  $\text{SO}_2$  and  $\text{O}_2$  to serve as a "fuel gas" in the indirectly-heated mode of operation. The subsequent thermal decomposition of  $\text{SO}_3$  is a reaction more amenable to indirectly heated reactors than is the decomposition of ferric sulfate. Sulfur trioxide will decompose over a broad temperature range, thereby providing for more compact heat exchangers operating at lower overall mean temperatures.

Further advantages accrue when one considers overall system reliability. If the ferric sulfate decomposition reactor were to be indirectly heated, inspection and maintenance of the heat exchange would require shutting down the entire process. Using a separate  $\text{SO}_3$  reduction reactor enables repair and maintenance to be conducted while the process continues to operate in the fuel gas mode.

The gases leaving the  $\text{SO}_3$  reduction reactor are cooled against the incoming stream and unreacted  $\text{SO}_3$  is condensed for recycle. Sulfur dioxide and oxygen sufficient to meet the thermal demands of the dryer and the ferric sulfate decomposition reactor are separated and rejoin the recycle to those vessels. The electrolyzer sulfur dioxide, with the process oxygen product, proceeds to the liquefaction cascade for separation. Sulfur dioxide recovered here is returned to the electrolyzer while the oxygen is a process by-product available for sale or disposal.



## 4.0 TECHNICAL AND ECONOMIC EVALUATION OF SELECTED HYDROGEN PRODUCTION PROCESSES

### 4.1 GENERAL

The hydrogen production processes selected for comparative technical and economic evaluations are:

- Water electrolysis, using Teledyne electrolyzers
- Coal gasification, using Bi-Gas two stage gasifiers
- Coal gasification, using Koppers-Totzek gasifiers
- Water decomposition, using the Westinghouse Sulfur Cycle

The bases for the selection of these systems were discussed in Section 3.0 of this report. The evaluation that is reported below attempts to present the technical and economic characteristics of each of these systems in a manner by which its potential for meeting the projected demands for hydrogen in the year 1985 and beyond can be assessed.

In order to prepare the necessary process flow sheets, mass and energy balances, and cost estimates for the various processes, a set of technical and economic ground rules had to be established. These ground rules were devised to make the comparisons between systems as straightforward as possible. The major general technical and economic ground rules applied to all systems are described below, while more detailed assumptions relative to individual systems are discussed in the report sections dealing with that system.

#### 4.1.1 Technical Ground Rules for Evaluation

The major technical ground rules for the evaluation of the hydrogen production systems are as follows:

- The plant product is a hydrogen stream with a purity of at least 95 volume percent. It is recognized that this ground rule will lead to results that are not truly comparable, since the purity of the hydrogen for water electrolysis and water decomposition will exceed 99 percent, while the purity of hydrogen from the coal based processes will be close to 95 percent. This disparity can be resolved by assuming an end use for the hydrogen and, if necessary, adding capital equipment and operating costs to upgrade the purity of the coal-derived hydrogen to that of the electrolytically produced hydrogen. Such an iteration is beyond the scope of this study.

- The plant product is assumed to be used off-site in an unspecified end use. Accordingly, a pipeline is included to the plant boundary and the product hydrogen is at a pressure suitable for feeding a pipeline, i.e., approximately 6900 kPa (1000 psi).
- Since the end use of the hydrogen is not specified, the practice of converting residual carbon monoxide and carbon dioxide to methane, to avoid potential health hazards in case of leakage, is adopted.
- By-product oxygen, if produced, is vented. For economic evaluations, a parametric credit for oxygen is assumed which would include the costs of "shipping" the oxygen off-site.
- The plant is located at the Middletown site described in NUS-531 (Reference 32).
- The plant design is based on a grass-roots facility, i.e., the plant is installed on a virgin site and is not an add-on to existing facilities.
- Although the Middletown site is specified, in Reference 32, to have adequate river water for cooling services, the plant design is based on the assumption that environmental concerns will preclude the use of anything other than cooling towers as a heat sink.
- Coal is assumed to be delivered to the plant site by rail, with the cost of coal including the cost of shipping.
- Electric auxiliary power is delivered to the plant site by 138 kV transmission lines. For the water electrolysis plant, where large bulk power supplies are required, it is assumed that the transmission lines are at 500 kV.
- The plants are designed to meet environmental protection regulations consistent with those in effect in early 1975.
- Ultimate disposal of waste is assumed to be off-site. On-site solid waste storage capability is used for temporary storage only.
- The plant designs assume that whatever R&D is required for successful operation has been successfully completed. The plant is not the first of a kind, but reflects an assumed mature technology.

#### 4.1.2 Economic Ground Rules for Evaluation

The major economic ground rules for the evaluation of the hydrogen production systems are as follows:

- All capital and operating costs are in July, 1974 dollars.
- No escalation has been included in the cost estimates. The sensitivity analysis of the effect of fuel or feedstock costs on the system does, of its nature, imply a certain rate of escalation.
- The economic analysis assumes private industry financing and tax rates.
- The annual fixed charge rate for depreciable capital investments is 15 percent for utility-type ownership and 25 percent for industrial-type ownership. The annual charge includes recovery of capital (profit, interest, and depreciation), Federal and State income taxes, local property taxes, interim replacements, and property insurance, as shown in Table 4.1.1.
- The annual fixed charge rate for non-depreciable and working capital is 10 percent.
- Interest rate during construction is 8 percent.
- The plant availability is 90 percent.
- The plant capacity factor is 80 percent.
- Nuclear fuel cost assumptions (materials, enrichment, reprocessing, etc.) for the very high temperature nuclear heat source are as shown in Table 4.1.2 and are identical to those used in Reference 1.
- The cost of coal includes the cost of shipping to the plant site.
- The cost of electric power, other than that generated on-site, is representative of the electric utility power rates for industrial customers.
- Cost estimates are based on the assumption that the plant is not the first of a kind, but is a developed mature type with no special non-recurring engineering or development costs associated with it. The cost of any necessary R&D is treated separately in the discussion of the technological status of the system.

TABLE 4.1.1

## ANNUAL CHARGE RATE ON DEPRECIABLE INVESTMENT

	<u>Utility</u>	<u>Industrial</u>
<u>Assumptions:</u>		
Plant Lifetime, Years (for economic write-off)	30.0	15.0
Percentage of Investment in Bonds	55.0	30.0
Interest Rate on Bonds, Percent	10.0	10.0
Return on Equity, Percent	10.0	15.0
Federal Income Tax Rate, Percent	48.0	48.0
State Income Tax Rate, Percent	3.0	3.0
Local Property Tax Rate, Percent	3.0	3.0
Interim Replacements Rate, Percent	0.35	0.35
Property Insurance Rate, Percent	0.25	0.25
<u>Annual Charge Rate, Percent:</u>		
Recovery of Capital		
Interest on Bonds	5.5	3.0
Return on Equity	4.5	10.5
Sinking Fund Depreciation	0.61	2.38
Federal Income Tax	1.28	4.70
State Income Tax	0.08	0.30
Local Property Tax	2.18	2.05
Interim Replacements	0.35	0.35
Property Insurance	<u>0.25</u>	<u>0.25</u>
Total, Percent	<u>14.8</u>	<u>23.5</u>
Total (Rounded Off), Percent	15	25

TABLE 4.1.2  
 NUCLEAR FUEL COST ASSUMPTIONS (VHTR)

<u>Item</u>	<u>Cost</u>
U <sub>3</sub> O <sub>8</sub> (natural uranium)	\$ 22.05/Kg (\$10/lb)
Conversion of U <sub>3</sub> O <sub>8</sub> to UF <sub>6</sub>	\$ 2.2/Kg (\$1/lb)
Separative Work	\$ 40/Kg
Reprocessing	\$ 170/Kg
Plutonium	\$9280/Kg
Thorium	\$ 9/Kg
Uranium-233	\$ 17,000/kg

## 4.2 WATER ELECTROLYSIS

### 4.2.1 General

The major item of technical and economic importance in a water electrolysis plant is the electrolyzer. Pressure electrolyzers were selected for this study because they have lower space requirements, lower product compression needs, and greater potential for reduction of specific power requirements than standard filter press or tank electrolyzers. Price quotations for electrolysis equipment indicated that vendor to vendor differences per unit of capacity would have little effect upon the conclusions reached in the study. Therefore, Teledyne HP modules were selected for the study to represent the technology and cost of water electrolysis equipment.

The cost of producing hydrogen is determined by system efficiency, the cost of equipment, and the cost of power. Very high system efficiencies can be obtained by operating the electrolyzers at low current densities and, consequently, low unit product outputs. In order to maintain an adequate production rate at the higher efficiency levels, more electrolyzers are needed and the plant cost rises. There is obviously a trade-off between operating efficiency, capital costs, and the cost of electrical power to arrive at an optimum electrolyzer design for a given set of economic conditions.

The overall efficiency of a water electrolysis plant is determined not only by the efficiency of the electrolyzers, but also by the efficiency of the conversion of thermal energy to electrical energy in the powerplant. By using electricity produced by a very high temperature nuclear reactor (VHTR) or by exotic systems, e.g., MHD, high conversion efficiencies can be achieved. Here again a trade-off exists between the efficiency level and the cost of achieving that level.

In the economic evaluation of hydrogen production by water electrolysis, no attempt was made to optimize the relationship between cost and efficiency. Operating conditions for the electrolyzers were based on vendor specifications for module operation at maximum capacity. In addition to the vendor's recommendation for the electrolyzers, the cost of power was based on today's least expensive means of generation electricity; i.e., utility owned light water nuclear powerplants.

The current technology used in the evaluation results in a 81.1 percent efficiency for the electrolyzer plant and a 34 percent efficiency for power generation. This gives a combined overall thermal efficiency for hydrogen production by water electrolysis of 27.6 percent. Supplying electricity by a VHTR with a combined high temperature Brayton cycle and a Rankine bottoming cycle would boost the power generation efficiency to perhaps 47 percent and raise the overall process efficiency accordingly to 38 percent. If, as some forecasters predict, efficiencies of 55 percent can be realized for power generation and over 90 percent for electrolysis cells (corresponding to an electrolyzer plant efficiency of about 88 percent), an ultimate overall efficiency for hydrogen production could be in the order of 48 percent - with an unidentified cost of development, capital, operation, and fuel. The quantification of costs for the extremely high efficiency water electrolysis plants and power supplies is beyond the scope of this present study.

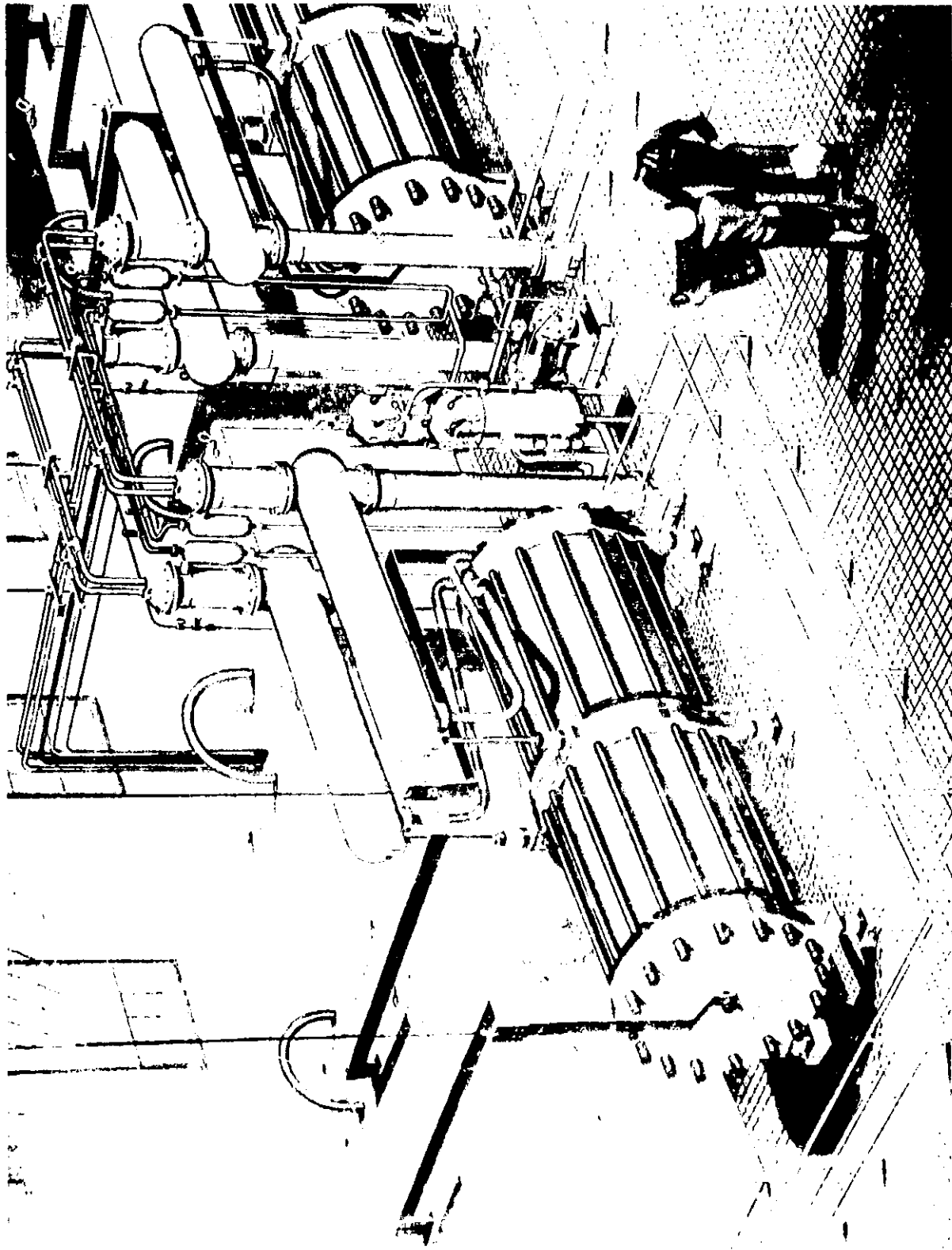


Figure 4.2.1 Eight Ton Per Day HP-Series Hydrogen Plant  
(Used with Permission of Teledyne Isotopes)

#### 4.2.2 Plant Design

The plant is capable of producing approximately  $9.4 \times 10^6$  std cubic meters per day of hydrogen. The plant design includes all the systems, structures, and facilities for the plant, but excludes the power generation facilities needed to meet the plant's electrical needs. The supply of electricity is assumed to be purchased power.

The large block of power required, in the order of 1720 MWe, would probably be supplied by one or more generating units "dedicated" to the hydrogen plant. For this reason, the generating units would be located as close as practicable to the hydrogen plant. Their construction can be expected to take longer than the time required to build the hydrogen plant, and the work on the power generation facilities would have to begin before the work on the hydrogen plant. However, both facilities can be developed independently of each other and constructed in parallel with identical scheduled completion dates. For purposes of economic evaluation, the power supply is assumed to be a two-unit light water nuclear power station providing electricity on an exclusive basis to the electrolysis plant. The sensitivity of the cost of hydrogen to the cost of electric power is also calculated and shown.

In order to provide a basis for the electrolysis plant cost estimates and for the evaluation of performance, a preliminary conceptual design was prepared. This design is described in the paragraphs below.

##### 4.2.2.1 Electrolyzers

Teledyne HP series modules (Reference 26) have been designed in capacities of 5000 to 40,000 std cubic meters of hydrogen per day. An 80,000 std cubic meter per day installation, consisting of two 40,000 std cubic meter per day modules is shown in Figure 4.2.1. For large plants, modules are packaged into "units." For this study, the vendor recommended that each "unit" consist of five 18,700 std cubic meter per day electrolyzers, the electrolyte separators, heat exchangers, electrolyte pumps and filters, demisters, dryers, instrumentation, and a common power supply. An installation consisting of 100 of these "units" is required to meet the total plant capacity.

The electrolyzers consist of individual cells, electrically in series, compressed together by tie rods. In each cell, the anode and cathode are separated by a gas impervious porous matrix electrolyte holder to prevent the product hydrogen and oxygen from mixing. The like gases from each cell are ducted internally through manifolds that bring the gases to a common point. Figure 4.2.2 shows a schematic of the basic system wherein the gases leave the cell together with entrained electrolyte and move through gas-liquid separators and heat exchangers. The separated electrolyte is returned through a filter to the electrolyzer module. Four pressure filter elements remove any foreign material that could block the narrow flow channels in the module. Any one of the four elements can be cleaned and returned to service without shutting the system down. Makeup feedwater is added on demand to the hydrogen/electrolyte separator, and its rate of addition is controlled by level switches in the separator. Level switches in both the hydrogen and oxygen separators also act as safety devices that will



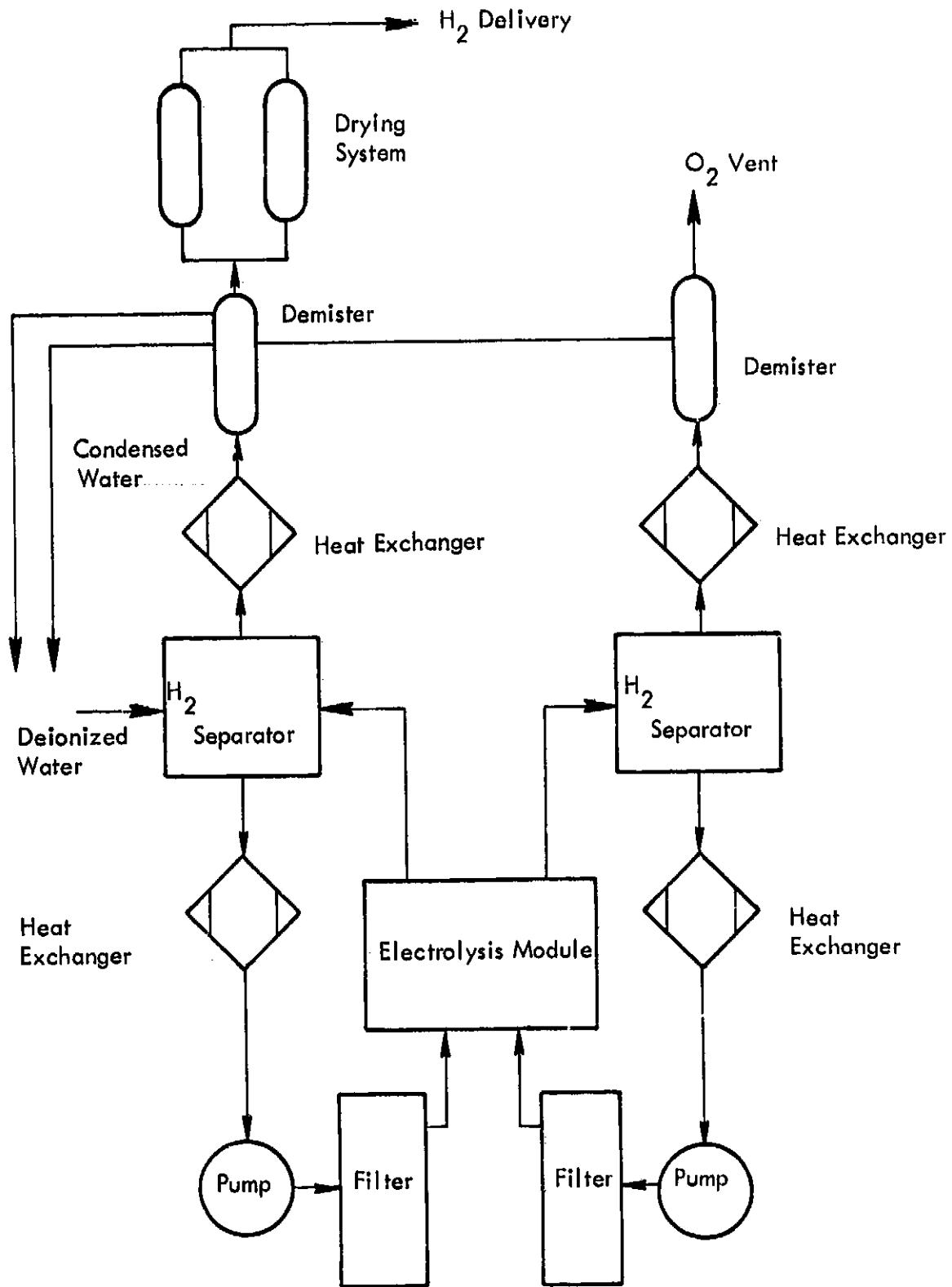


Figure 4.2.2 System Schematic, Teladyne HP Modules  
 (Used with Permission of Teledyne Isotopes, Timonium, MD)

shut the system down if abnormally high or low levels exist. Both separators are also equipped with high pressure alarms and relief valves.

The heat generated by system inefficiencies is removed from the electrolyte by water cooled heat exchangers. The cooling water flow of about  $0.058 \text{ m}^3/\text{std m}^3 \text{ H}_2$  (77.2 gal/lb  $\text{H}_2$  or 0.43 gal/SCF  $\text{H}_2$ ) is controlled to maintain the desired outlet temperature. The temperature and flow of the electrolyte are monitored continuously, and a temperature monitor sounds an alarm if an abnormally high temperature condition exists. The high temperature condition may be temporarily alleviated by increasing the cooling water flow; but if the over-temperature persists and a critical temperature is reached, the temperature monitor will stop power to the module. If a normal temperature is not reached within ten minutes, the gas lines are purged with nitrogen and the entire system cooled and shut down.

The gases are cooled to room temperature in water cooled heat exchangers and passed on to a demister where most of the condensed water of saturation is collected and returned to the makeup feedwater system. In this study, the oxygen is considered to be of no value and is vented at this point. However, an oxygen delivery system can be provided and is analogous to the hydrogen system to be described. The hydrogen delivery system of the Teledyne HP units provides a combination molecular sieve and catalyst purification system that dries the hydrogen to a dewpoint below 205K ( $-68^\circ\text{C}$ ) and removes traces of oxygen. Particles entrained by the gas in the drying columns are removed by a final dust filter so that the product hydrogen has a purity of better than 99.99 percent. Typical impurities present in amounts less than 0.2 ppm (by volume) are oxygen, water vapor, hydrocarbons, and nitrogen.

The hydrogen product exits as a high purity gas at 690 kPa (100 psi) and is compressed to 6895 kPa (1000 psi) for pipeline delivery. An overall mass balance for the electrolysis plant is shown in Table 4.2.1, with the corresponding energy balance shown in Table 4.2.2.

Stainless steel is used for all vessels and piping. The equipment is designed as small as possible to minimize gas hold-up and capital cost. Maintenance is minimized by using magnetic drive pumps instead of conventionally packed pumps. Control loops have automatic backup and manual override systems. Manual operation is possible from a central control panel, and recorders provide a process history. However, the systems are completely automatic, and many units may be monitored and/or operated from a central control room.

#### 4.2.2.2 Plant Subsystems

In addition to an electric powerplant, various subsystems are required to support the operation of the electrolyzer modules. These include the primary water treatment, feedwater purification, and storage system; the electrolyte preparation and storage system; the heat removal system for the plant; the product gas handling system; and the electric auxiliary power system.

These subsystems, together with the basic electrolyzer module packages and buildings, comprise the essential elements of a large electrolysis plant. A flow sheet relating these systems, one to the other, is shown in Figure 4.2.3.

TABLE 4.2.1  
 OVERALL MASS BALANCE FOR THE PRODUCTION OF  $9.4 \times 10^6$  STD  $m^3$  HYDROGEN PER DAY

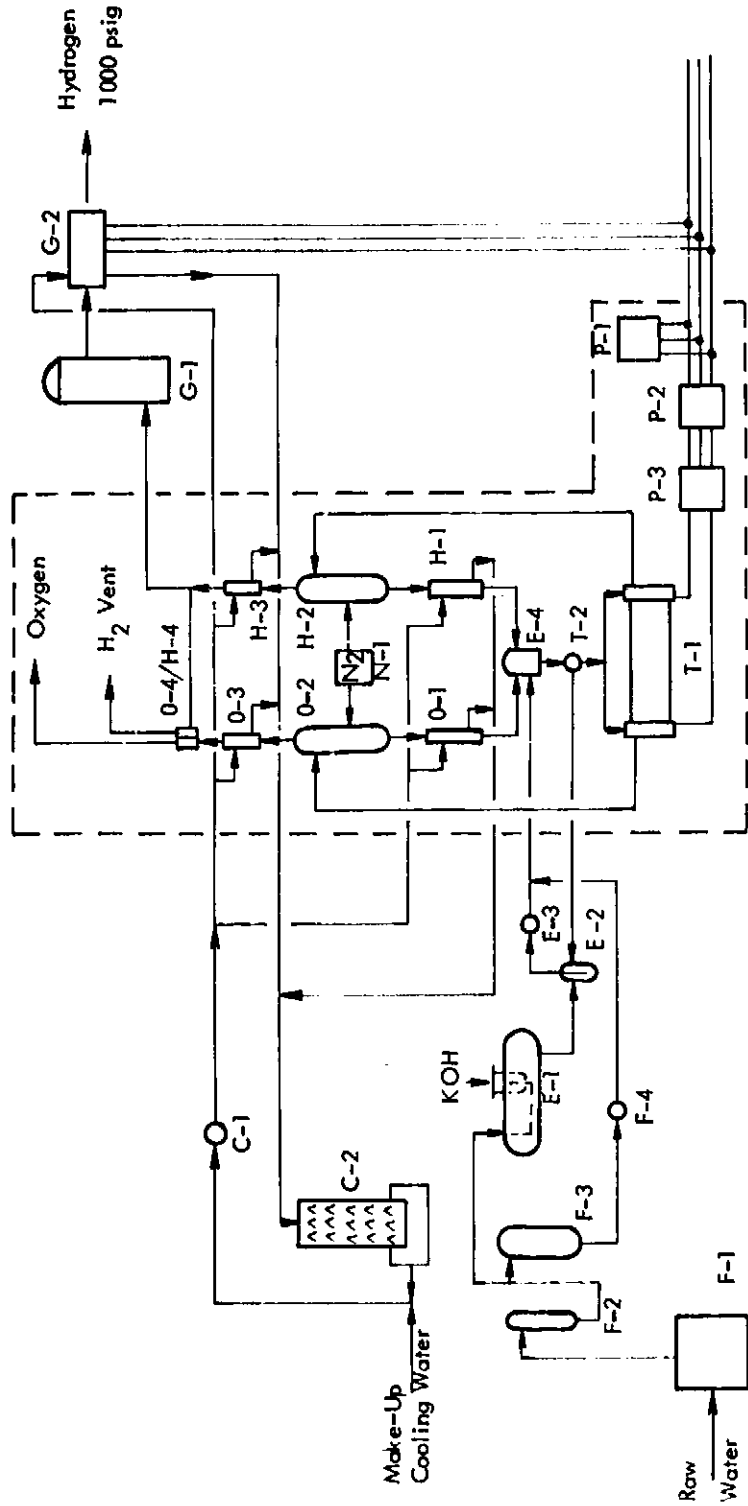
NOTE: An initial charge of  $4.8 \times 10^6$  kg ( $10.6 \times 10^6$  lbs) of potassium hydroxide in  $14.4 \times 10^6$  kg ( $31.7 \times 10^6$  lbs) of water is retained in the system.

Item	Input		Output	
	1000 kg/hr	1000 lbs/hr	1000 kg/hr	1000 lbs/hr
<b>Electrolyzers</b>				
Feedwater	319	702	-	-
Hydrogen (690 kPa)	-	-	35	78
Oxygen (690 kPa)	-	-	284	624
Subtotal	319	702	319	702
<b>Compressor Station</b>				
Hydrogen (690 kPa)	35	78	-	-
Hydrogen (6895 kPa)	-	-	35	78
<b>Cooling Towers</b>				
Water from Electrolyzers	22,718	49,980	-	-
Water from Compressors	1,122	2,469	-	-
Make-Up Water	1,175	2,584	-	-
Air (Dry Basis)	390,182	858,401	390,182	858,401
Water Vapor in Air	4,791	10,541	5,966	13,125
Cooling Water	-	-	23,840	52,449
Subtotal	419,988	923,975	419,988	923,975
<b>Total</b>	420,342	924,755	420,342	924,755

TABLE 4.2.2

OVERALL ENERGY BALANCE FOR THE PRODUCTION OF  
 $9.4 \times 10^6$  STD  $m^3$  HYDROGEN PER DAY

<u>Item</u>	<u>Energy (<math>10^6</math> Joules/Second or Megawatts)</u>	
	<u>Input</u>	<u>Output</u>
<b>Electrolyzer</b>		
Water Enthalpy	4.7	-
Power Input	1,666.1	-
Hydrogen Enthalpy	-	1.8
Oxygen Enthalpy	-	0.5
Decomposition Enthalpy	-	1,411.0
Heat Loss	-	257.5
Subtotal	1,670.8	1,670.8
<b>Pumps and Compressor Station</b>		
Estimated Input to Pumps	13.8	-
Estimated Input to Compressors	32.3	-
Hydrogen Enthalpy (690 kPa)	1.8	-
Work of Pumping	-	6.9
Hydrogen Enthalpy (6895 kPa)	-	18.1
Heat Loss	-	22.9
Subtotal	47.9	47.9
<b>Cooling Towers</b>		
Water Enthalpy	1,582.9	-
Make-Up Enthalpy	40.2	-
Moisture Enthalpy in Air	0.4	0.1
Air Enthalpy	8,577.0	9,366.9
Heat Loss	-	18.0
Water Enthalpy	-	815.5
Subtotal	10,200.5	10,200.5
Total	11,919.2	11,919.2



<u>Feedwater System</u>	<u>Electrolyte System</u>	<u>Electrolysis Gas Modules</u>	<u>Power Conditions</u>
F-1 Water Treatment Plant	E-1 Electrolyte Tank	O-1 Heat Exchanger	P-1 Process Controls
F-2 Ion Exchanger	E-2 Suction Drum	O-2 Gas/Electrolyte Separator	P-2 Transformer
F-3 Feedwater Tank	E-3 Electrolyte Pump	O-3 Condenser	P-3 Bridge Rectifier
F-4 Feedwater Pump	E-4 Electrolyte Filter & Mixer	O-4/H-4 Pressure Controller	
		H-1 Heat Exchanger	<u>Hydrogen Service</u>
<u>Cooling Water</u>	<u>Electrolysis Cell Module</u>	H-2 Gas/Electrolyte Separator	G-1 Low Pressure Gas Storage
C-1 Cooling Water Pump	T-1 Electrolysis Cells	H-3 Condenser	G-2 Compressor Station
C-2 Cooling Tower	T-2 Electrolyte Feed Pump		

Note: Basic Equipment Supplied by Vendor is Enclosed by Dashed Lines

Figure 4.2.3 Process Flow Diagram for a Water Electrolysis Plant

Table 4.2.3 shows the services required for the operation of a single electrolyzer module, a five module unit operating from a common power supply, and for the total plant consisting of the 100 five module units capable of producing  $9.4 \times 10^6$  std cubic meters of hydrogen per day.

#### 4.2.2.3 Water Make-Up System

Raw river water is taken to the water treatment plant to provide the make-up cooling water and feedwater required for plant operation. A pumphouse, located at the river, contains the raw water pumps and the trash rakes and traveling screens needed to keep the make-up water free from debris.

The raw water is treated by coagulation and filtration to make it suitable as feed to the fire protection system, sanitary system, general plant services, and the make-up feedwater demineralization system. In the demineralization system, the clarified and filtered water is passed, in series, through cation exchangers, degasifiers, anion exchangers, and a final treatment in mixed bed ion exchangers to result in a minimum resistance of 50,000 ohm/cm. The purified water is stored in a stainless steel tank and is used to supply water to dissolve electrolyte or to the electrolysis modules as required.

#### 4.2.2.4 Electrolyte Preparation and Storage System

An electrolyte tank is used to prepare the electrolyte solution (a 25 percent by weight solution of potassium hydroxide) for use as needed and to serve as a holding tank for the solution when electrolyzer modules are taken out of service for maintenance or repair. The initial charge for a single HP electrolyzer module is  $27.6 \text{ m}^3$  (7300 gals) of 25 % KOH solution. The potassium hydroxide must be of good quality and free of metal ions and organic matter. The potassium hydroxide and deionized water are agitated in the mixing tank and pumped through the cells and filters until a clear, homogeneous solution is obtained. Nitrogen can be used to purge the system of air and prevent absorption of carbon dioxide by the electrolyte.

#### 4.2.2.5 Heat Removal System

To minimize the potential environmental impact of the plant, cooling towers are used for ultimate heat rejection. These result in higher capital and operating costs than direct river cooling, but avoid the concerns with thermal discharges to the waterway.

The wet natural draft cooling towers transfer heat to the air by a combination of sensible heat transfer and evaporative cooling. The water make-up system must provide sufficient replacement water to compensate for the evaporative, windage, and blowdown consumption.

TABLE 4.2.3  
SERVICES REQUIRED

	<u>Module</u>	<u>Unit</u>	<u>Plant</u>
Deionized Water, m <sup>3</sup> /hr	0.64	3.19	319
, Gal/min	2.82	14.05	1,405
Cooling Water , m <sup>3</sup> /hr	45.4	227.0	22,710
, Gal/min	200.0	1,000.0	100,000
Total Electrolyzer Power, MWe	3.3	16.7	1,666
Pumps	←———— 440 V, 3φ —————→		
Other	←———— 220 V, 3φ —————→		
Air	← Oil Free Compressed Air, 80 psig →		
Nitrogen			
Start-Up, std m <sup>3</sup>	3.75	18.8	2,100
, SCF	140	700	78,400
Emergency, std m <sup>3</sup>	113	563	63,000
, SCF	4200	21,000	2,352,000
Potassium Hydroxide, 25 w/o			
Initial Filling, m <sup>3</sup>	27.6	138	1,547
, Gal	7300	36,500	4,088,000

#### 4.2.2.6 Product Gas Handling

Hydrogen is produced in the electrolyzers at a pressure of 690 kPa (100 psi). It has been assumed that the product gas is used off-site, in some unspecified process that feeds off a hydrogen pipeline. A compressor station is included in the hydrogen generation plant to provide the 6895 kPa (1000 psi) pressure for the pipeline delivery. Included in the station are gas storage tanks to provide a suction-side working inventory and surge capacity for the compressors.

#### 4.2.2.7 Electrical Auxiliary Power System

The electrical auxiliary power system provides the facilities to distribute power to the electrolyzer unit common power supplies and to all other process equipment in the plant. All electric power is generated outside the hydrogen production plant fence. As a base case assumption, it is considered that the power requirements are met by a two-unit light water nuclear power station adjoining the hydrogen plant site, with power being transmitted by 22 kV isolated phase bus duct. If the power generation facilities are remote from the hydrogen plant, power would be accepted at the switchyard from a 500 kV transmission line.

#### 4.2.2.8 Plant Maintenance

The electrolyzer units are totally automatic and controlled from a central control room. The need for operational maintenance would be identified in the control room by signals from monitoring instrumentation. Routine maintenance consists of changing filters, inspections, instrumentation calibration, and the like. A preventive maintenance schedule for a typical small hydrogen plant is shown in Table 4.2.4. In a large plant, the electrolyte would probably not be changed semi-annually, but only when sample analysis indicated the need for a change. The discharged electrolyte would in most cases be processed for re-use.

### 4.2.3 Plant Performance Characteristics

The performance of the plant can be expressed in several ways. The paragraphs below summarize the performance in terms of resource consumption, process outflows, and overall thermal efficiency. The performance, relative to other hydrogen production processes, is summarized in Section 5.

#### 4.2.3.1 Resource Consumption

For purposes of evaluation, the only resources considered are those associated with the operation of the plant and not with the manufacture or construction of the facility. Table 4.2.5 summarizes the annual resource consumption for hydrogen production at an 80 percent plant capacity factor. In addition to the water requirements given in Table 4.2.1, the plant consumes ion exchange resin, potassium hydroxide, nitrogen, and various other chemicals and miscellaneous materials. Only the major resources are shown in Table 4.2.5 and are based on a number of assumptions. Ion exchange resins are assumed to be changed and discarded twice



TABLE 4.2.4

PREVENTATIVE MAINTENANCE SCHEDULE, TELEDYNE HP MODULES

Assumes 3 Shift 24 Hour Operation of Plant

	1	2	3	4	5	6	7	8	9	10	11	12	13
Preventative													
Maintenance													
Month	730	1460	2190	2920	3650	4380	5110	5840	6570	7300	8030	8760	9500+
Hours													
Electrolyte Sample	x	x	x	x	x	x	x	x	x	x	x	x	Monthly
Electrolyte Change	x					x						x	Semi-Annually
Electrolyte Filter Element Inspection	x		x			x						x	Semi-Annually
Product Gas Filter Inspection						x						x	
Valve Maintenance	x					x						x	Semi-Annually
Pump Bearing Inspection												x	Annually
Pressure Switch Calibration						x						x	Semi-Annually
Module Assembly	x					x						x	Semi-Annually
Instrument Calibration						x						x	Semi-Annually
Test and Calibration of Safety Instrumentation	x		x			x			x			x	Quarterly

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TABLE 4.2.5

WATER ELECTROLYSIS

ANNUAL RESOURCE CONSUMPTION

(80% Capacity Factor)

Electricity		
• Electrolysis		$117.0 \times 10^8$ KWH
• Pumps, Compressors, Etc.		$3.4 \times 10^8$ KWH
Cooling Water Make-Up		$8.2 \times 10^9$ kg ( $18.1 \times 10^9$ Lbs)
Deionized Water		$2.2 \times 10^9$ Kg ( $4.9 \times 10^9$ Lbs)
Ion Exchange Resins		$22.7 \text{ m}^3$ (800 Cubic Feet)
Potassium Hydroxide		$4.5 \times 10^4$ Kg ( $10.0 \times 10^4$ Lbs)
Nitrogen		$66.3 \times 10^3 \text{ m}^3$ ( $2340 \times 10^3$ SCF)

a year. Potassium hydroxide, after an initial filling of the electrolyzers, is required to replace stack (oxygen venting) and reprocessing losses at an estimated rate of  $4.5 \times 10^4$  kg/year (100,000 lb/yr). About  $2.2 \times 10^3$  std m<sup>3</sup> (78 MSCF) of nitrogen is used in the initial filling of the electrolyzers to prevent the electrolyte from absorbing carbon dioxide from the atmosphere. Nitrogen is kept on hand for emergency use and also for use during electrolyte transfers and reprocessing operations. The annual use of nitrogen has been taken as equal to the amount kept in storage.

The resource impact of the electric power consumed would be a factor of the type of powerplant ultimately used to supply the energy and therefore it is not specified in more detail in the table.

#### 4.2.3.2 Process Outflows

The products of the process operation, in addition to the hydrogen stream, include a myriad of other flows. The major outflows, on an annual basis, are shown in Table 4.2.6. It should be noted that the oxygen stream is categorized as a waste only because it was assumed that all the oxygen was to be vented from the plant. Depending upon needs and logistics of distribution, the oxygen can perhaps be a product of value which can be sold.

#### 4.2.3.3 Process Thermal Efficiency

Whereas Table 4.2.2 shows an energy balance around the different components of the hydrogen plant, Table 4.2.7 shows a summary that gives the overall operating efficiency of the plant. On the basis of the total electric power input, the plant is 81.1 percent efficient. However, if the thermal efficiency of the light water nuclear powerplant, used for the base case economic evaluation, is taken into account at an assumed 34 percent level, the overall thermal efficiency for the production of hydrogen by water electrolysis drops to 27.6 percent.

The efficiency of electrolyzers is affected by the operating conditions. Higher hydrogen production rates are obtained by operating modules at higher current densities, but with some loss of operating efficiency. The hydrogen plant for this study is based on hydrogen production at the maximum capacity of the recommended Teledyne HP modules. No further effort was made to optimize equipment usage or operating efficiency based on changes in operating conditions, but instead the equipment was accepted as typical of the current state-of-the-art.

Similarly, the efficiency of electric generation can be increased at additional cost. Light water nuclear reactors provide the least expensive electric generation costs, at efficiency levels of about 34 percent. Current technology fossil fueled powerplants can produce electricity at efficiencies of 36 to 40 percent, with power costs higher than nuclear. Advanced power generation systems are projected with efficiency levels of 50 percent and more, but with unknown development, capital, and fuel costs. The ultimate efficiency of water electrolysis plants will depend on the results of development programs yet to be performed and the optimization, in respect to cost and energy effectiveness, of the combined power generation/electrolysis plant.

TABLE 4.2.6

WATER ELECTROLYSIS

ANNUAL PROCESS OUT FLOW  
(80% Capacity Factor)

Product	$2.74 \times 10^9 \text{ m}^3$ ( $10.24 \times 10^{10}$ SCF)
Waste Streams	
Oxygen	$1.37 \times 10^9 \text{ m}^3$ ( $5.12 \times 10^{10}$ SCF)
Nitrogen	$6.9 \times 10^4 \text{ m}^3$ ( $2.43 \times 10^6$ SCF)
Ion Exchange Resins	$22.7 \text{ m}^3$ (800 Cubic Feet)
Solids (from filtration systems)	$2.2 \times 10^4 \text{ Kg}$ (24 Tons/Year)
Potassium Hydroxide (Estimated Stack and Reprocessing Losses)	$4.5 \times 10^4 \text{ Kg}$ (50 Tons/Year)

TABLE 4.2.7

WATER ELECTROLYSIS

OVERALL EFFICIENCY

Heat Inputs	
Electrical	1712 MWe ( $5.85 \times 10^9$ Btu/Hr)
Thermal ( $MW_e/MW_T = 0.34$ )	5035 MWt ( $17.2 \times 10^9$ Btu/Hr)
Heat Outputs	
Product Gas	$2.74 \times 10^9$ Std $m^3$ /Yr ( $10.24 \times 10^{10}$ SCF/Yr)
Heating Value	3.55 kWh/Std $m^3$ (325 Btu/SCF)
Total Heat Output	1388 MWt ( $4.75 \times 10^9$ Btu/Hr)

Process Efficiency (Electrical)

$$\frac{1388 \times 100}{1712} = 81.1\%$$

Overall Efficiency (Thermal)

$$\frac{1388 \times 100}{5035} = 27.6\%$$

#### 4.2.4 Economics

An evaluation of the economics of hydrogen production by water electrolysis is important because it forms the basis for comparison with other methods of hydrogen production. Water electrolysis is the most straightforward and "cleanest" method of producing hydrogen, but large-scale production by this route is heavily dependent upon the cost of electrical power. Hydrogen, produced by water electrolysis during off-peak demand hours, has been suggested as an energy storage medium that can, if necessary, be converted back to electricity during peak demand periods by fuel cells or turbines. However, a discussion of this is outside the scope of this study. For the purpose of this report, hydrogen is produced as an item of commerce using power from adjacent generating facilities. The cost of power is treated as an important variable in the initial cost analysis, but the impact of providing captive power and absorbing the capital cost of the powerplant in order to reduce the overall power costs is also discussed.

In determining the hydrogen production cost, estimates were made of the capital, operating and maintenance, and power costs for the facility in the general format used in reporting nuclear powerplant costs, as defined in NUS-531 (Reference 32). The effects on production costs of different capacity factors, power costs, and type of ownership were also considered.

##### 4.2.4.1 Capital Costs

The capital costs are based on preliminary sizing of most of the major plant equipment and determining appropriate costs for that equipment. Factors, based on experience, were used to account for the costs of installation, piping, valves, instrumentation, structures, and miscellaneous equipment. Indirect costs were also estimated by applying factors in the manner described below.

The electrolysis plant is estimated to require a direct cost investment, in mid-1974 dollars, of \$351,462,000, as shown in Table 4.2.8. The direct cost is presented according to a code of accounts that divides systems among on-sites and off-sites, with the former relating to closely related mainline processing steps and the latter consisting of support and service systems and facilities.

The Teledyne HP electrolyzer modules are the major cost component of the plant. They are complete systems and include separators, heat exchangers, electrolyte pumps, demisters, dryers, instrumentation, and power conversion equipment. Since they are purchased as packaged units, installation costs and engineering services are minimized.

The total plant investment, shown in Table 4.2.9, includes the direct costs plus contingencies, indirect costs, and interest during construction. For the purpose of evaluation, land and land rights are shown separately from other direct costs since it is a nondepreciating asset.

TABLE 4.2.8  
 WATER ELECTROLYSIS PLANT  
 DIRECT CAPITAL COSTS  
 (July 1974 Dollars)

<u>Account</u>	<u>Item</u>	<u>Installed Cost ( \$ Thousands)</u>
<u>2000</u>	<u>On-Sites</u>	
2100	Electrolyzer Power Supply	\$(included in 2200)
2200	Electrolyzer System and Building	291,218
2300	Electrolyte System	1,094
2400	Hydrogen Product Compression	<u>19,160</u>
	On-Sites Subtotal	\$311,472
<u>1000</u>	<u>Off-Sites</u>	
1100	Cooling Water System	\$ 4,562
1200	Make-Up and Feedwater System	9,557
1300	Waste Water Treatment	300
1600	Electrical Auxiliary Power	19,600
1700	General Off-Sites Investment	
1710	Land and Land Rights	800
1720	Site Improvements and Facilities	1,500
1730	Administration/Service/Laboratory Buildings	1,100
1740	Instrument and Plant Air	500
1750	Maintenance Facilities	900
1760	Fire Protection, Communications	846
1770	Furnishings, Fixtures, Laboratory Equipment	<u>325</u>
	Off-Sites Subtotal	\$ 39,990
	Total Direct Capital Cost	\$351,462

Special materials comprise the initial supply of potassium hydroxide, resins, and other materials needed for operation of the plant. A contingency of 15 percent is applied, for the hydrogen generation facilities, to the estimated cost of the special materials and the direct cost of the physical plant.

Indirect costs are expense items of a general nature which apply to the overall project of building an operable plant, rather than to one of the direct costs. These costs, except for interest during construction, have not been estimated in detail, but calculated as a percentage of the direct costs based on the procedure defined in NUS-531.

Construction facilities, equipment, and services include general costs associated with the plant construction, such as field offices, warehouses, temporary power and utility lines, cost or rental of construction equipment and supplies, purchase of electric power, water, and other utilities, security guards, training programs for the labor force, inspection and testing of construction materials, site cleanup, insurance, and the like.

Engineering services include items such as preliminary investigations; site selection; air and water environmental studies; subsurface investigations; preparation of specifications and evaluation of proposals for major equipment packages, preparation of preliminary and final design documents, design reviews, procurement, inspection, and expediting of materials and equipment; preparation of pre-operational test and plant startup procedures; assistance in securing plant permits; management and direction of construction activities, including selection of subcontractors, scheduling, maintaining cost and quality control; on site procurement and receiving of materials and equipment; field accounting; supervising and pre-operational testing of systems and components; field engineering inspection of construction work to assure compliance with plans and specifications; and preparation of as-built drawings. A significant part of the systems engineering of the plant is included in the cost quotation for the electrolyzer units.

Other costs include the owner's property and all-risk insurance, state and local property taxes on the site and improvements during construction, sales taxes on purchased materials and equipment, staff training, plant startup, and the owner's general and administrative (G&A) costs.

Interest during construction is calculated as simple interest, at an 8 percent annual rate, on the plant investment as it is made. For the purpose of the evaluation, it is assumed that the land is purchased six months prior to the start of the project and that special materials are delivered and paid for nine months prior to plant commercial operation. The remainder of the plant investment is made as design and construction proceeds over a four year period as shown in Figure 4.2.4. Inherent in this curve is an initial two year period in which expenditures remain reasonably low while engineering proceeds, environmental impact statements are prepared, and permits for construction are solicited.

The total plant investment, including all direct and indirect costs, but excluding escalation and the cost of the power generation plant, is estimated to be \$505,393,000 for the grass roots facility.



TABLE 4.2.9  
 WATER ELECTROLYSIS PLANT  
 ESTIMATED CAPITAL COST SUMMARY  
 (In Thousands of Dollars)

Non-Depreciating Assets		\$ 800
Land and Land Rights		
Depreciating Assets		
Special Materials	1,933	
Physical Plant	<u>351,462</u>	
	\$353,395	Subtotal
Contingency	<u>53,009</u>	
	\$406,404	Subtotal
Indirect Costs		
Construction Facilities, Equipment and Services	\$ 22,356	
Engineering Services	19,100	
Other Costs	13,414	
Interest During Construction	<u>43,319</u>	
Indirect Costs	\$ 98,189	
Total Depreciating Assets	\$504,593	
Total Plant Investment	\$505,393	

#### 4.2.4.2 Operation and Maintenance Costs

The costs of operation and maintenance includes the expense of maintaining a plant staff, consumable supplies and equipment, outside support services, miscellaneous items of cost, and indirect costs of maintaining the plant working capital.

The direct O&M costs are shown in Table 4.2.10. The staff costs are based on a 70 person staffing level, at an average cost of \$19,300 per man-year. The costs of chemicals and catalysts are based on their assumed use rate. An allowance of \$300,000 has been included for miscellaneous consumables.

Outside support services are taken to embrace all services obtained other than from the normal plant complement during normal working hours. Other requirements for outside support services include such items as off-site disposal of wastes, major equipment overhauls, and consultants to provide various forms of operational support.

Miscellaneous O&M costs include such items as training new staff personnel; requalification of operators; rent for property, equipment, or facilities which are used or occupied in connection with plant operation; travel, such as to staff conferences at the main office or to professional society meetings or other conferences; licenses and fees; office supplies, postage, and telephone/telegaph bills; and fuel and upkeep of station vehicles.

The total direct annual operation and maintenance cost of \$2,239,000 includes a 15 percent G&A assessment on all costs.

The indirect O&M costs are shown in Table 4.2.11. These are the costs of maintaining the working capital required for continued operation of the plant and is evaluated at a 10 percent annual charge rate. The working capital is made up of the cash in hand needed to meet the day to day operating expenses plus the value of materials and supplies in inventory. The average net cash required is calculated at 2.7 percent of the direct O&M costs. A two month supply of consumables is assumed to be kept in inventory.

The total O&M costs, at a plant capacity factor of 80 percent, are shown in Table 4.2.12.

#### 4.2.4.3 Power Costs

Power requirements for the hydrogen plant are very large. The power generation facilities are not considered as part of the electrolysis plant - all electric energy is assumed to be purchased. Several different approaches can be used to determine the annual cost of power. One assumes that the power is drawn from an electric utility transmission network and paid for at the rates that utilities charge their industrial bulk users. This approach, for the base case economics, would result in power costs of about 2¢/kwh - a reasonably typical cost for mid-1974 bulk power purchases.

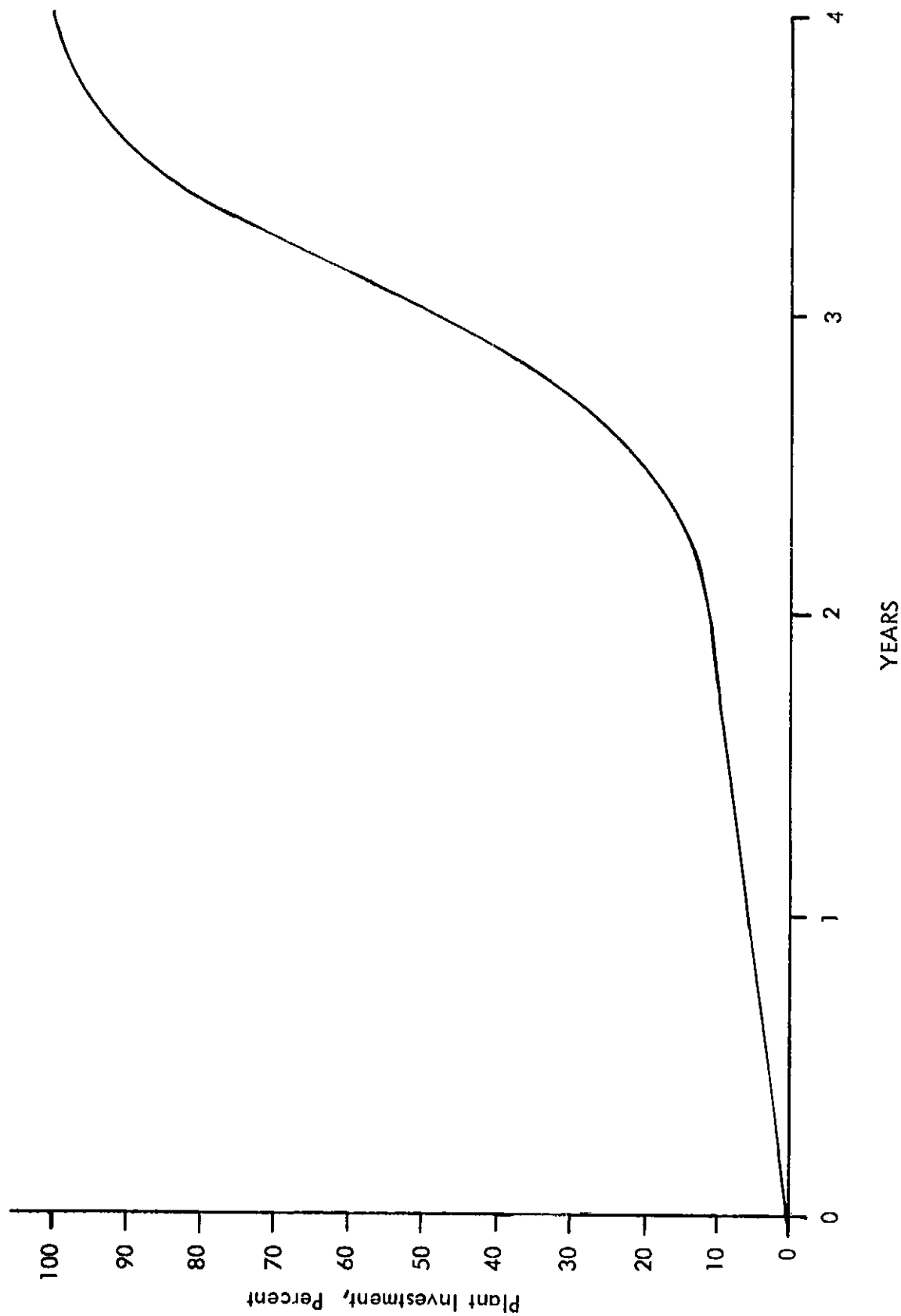


Figure 4.2.4 Water Electrolysis - Plant Capital Investment Expenditures Versus Time

TABLE 4.2.10

WATER ELECTROLYSIS

DIRECT ANNUAL O & M COSTS

Staff Payroll		
70 People		\$ 1,351,000
Consumable Supplies and Equipment		
Chemicals and Catalysts	75,000	
Miscellaneous (Lubricants, Maintenance Materials, Filters, Gaskets, Etc.)	<u>300,000</u>	
		\$ 375,000
	Subtotal	
Outside Support Services		
Ultimate Disposal of Solid Wastes	1,000	
Contracted Work, Consultants, Etc.	<u>140,000</u>	
		\$ 141,000
	Subtotal	
Miscellaneous		
Training, Travel, Office Supplies, Etc.	<u>80,000</u>	
		\$ 1,947,000
	Subtotal	
G & A		
		<u>292,000</u>
	Total Direct O & M Costs	\$ 2,239,000

TABLE 4.2.11  
 WATER ELECTROLYSIS  
 INDIRECT OPERATION AND MAINTENENCE COSTS

Average Net Cash Required	\$ 60,000
Materials and Supplies In Inventory	
Consumable Supplies and Equipment	<u>63,000</u>
Total O & M Working Capital	\$ 123,000
Annual Charge Rate	10%
Annual Indirect O & M Cost	\$ 12,300

TABLE 4.2.12  
 WATER ELECTROLYSIS  
 TOTAL ANNUAL O & M COSTS  
 (80% Capacity Factor)

	<u>Cost</u>
Direct O & M Costs	\$ 2,239,000
Indirect O & M Costs	<u>12,300</u>
Total	\$ 2,251,300

The other approach assumes that the power is supplied by a dedicated nuclear power station located adjacent to the electrolysis plant to avoid transmission costs. Such a plant, if it used light water nuclear reactors (PWR or BWR), could produce electricity at a cost significantly less than the cost of purchased power from the utility grid. The nuclear station would contain two 860 MWe units and, according to Reference 33, would have a capital cost, in mid-1974 dollars, of about \$822, 160, 000. If a power cost evaluation is made, following the procedure of NUS-531 (Reference 32), the costs shown in Table 4.2.13 result. Two alternate types of ownership are presumed; i.e., industrial, with a 25 percent annual charge on capital, and utility-type, with a 15 percent annual charge. Operation and maintenance costs include staffing, materials, services, working capital charges, and nuclear insurance. Fuel costs represent typical water reactor fuel cycle expenses of about 19.9¢/GJ (21¢/10<sup>6</sup> Btu). The resultant power costs would range from 1.28¢/kwh for the utility type of ownership to 1.96¢/kwh if the powerplant were owned by a non-regulated industrial organization. This can be compared to the 2¢/kwh expected purchased power cost from a utility system, which draws upon a mixture of nuclear and fossil fired units and includes the allocated costs of transmission.

The annual cost of power to the electrolysis plant, as a function of the source of electricity, is shown in Table 4.2.14 for the base case economic assumptions.

#### 4.2.4.4 Hydrogen Production Costs

The hydrogen production power cost is made up of the contributions of capital, operation and maintenance, and power costs. These are normally calculated on an annual basis. The percentage of the plant investment that is charged against production each year is a fraction of the type of plant ownership; i.e., utility or industrial, and the manner in which the owner can do business. As discussed in Section 4.1.2, the annual charge on non-depreciating assets; e.g., land, is 10 percent for either type of ownership while the annual charge on depreciating assets is 15 percent for utility ownership and 25 percent for industrial ownership. Although production costs are calculated on both a utility and industrial basis, it is not realistic to consider that the production of hydrogen, on the scale contemplated and with distribution to remote "users", would be an "industrial" enterprise. It is considered that this sort of production plant would much more readily fit a "regulated utility" type of enterprise — much like today's natural gas and electrical utility operations.

The cost of hydrogen production, on both bases, is shown in Table 4.2.15. A dedicated nuclear plant is considered as the power source, with its power cost also being a function of utility or industrial ownership. As can be seen, the cost, which is equivalent to a "gate selling price," is 8.47¢ standard m<sup>3</sup> (\$2.27/MSCF), or \$6.62/GJ (\$6.98/10<sup>6</sup> Btu) on a utility basis. The cost to the ultimate consumer would be this production cost plus the allocated capital and operating costs of transmission and distribution.

#### 4.2.4.5 Sensitivity of Hydrogen Production Costs to Variables

The cost of hydrogen production from any given plant will vary with the cost of fuel, the type of ownership, and the utilization; i.e., capacity factor, of the facility. For a base

TABLE 4.2.13  
 WATER ELECTROLYSIS  
 ESTIMATED POWER COSTS - DEDICATED NUCLEAR POWER STATION  
Rating - 1720 MWe  
(80% Capacity Factor)

	(Thousands of Dollars/Year)	
	<u>Utility Owned Power Station</u>	<u>Industrially Owned Power Station</u>
Capital (\$822,160,000)	\$123,324	\$205,540
Operation + Maintenance	5,350	5,350
Fuel	25,284	25,284
Total Annual Cost	\$153,958	\$236,174
Power Cost	1.28¢/kwh	1.96¢/kwh

TABLE 4.2.14  
 WATER ELECTROLYSIS - ANNUAL POWER COST  
 (80% Capacity Factor)

	<u>Purchased Power</u>	<u>Dedicated Nuclear Power Station</u>	
		Utility Owned	Industrial Owned
Power Cost	\$.02/kwh	\$0.0128/kwh	\$0.0196/kwh
Total Cost	\$240,800,000	\$153,958,000	\$236,174,000

TABLE 4.2.15  
 WATER ELECTROLYSIS  
 HYDROGEN PRODUCTION COST COMPARISON  
 (80% Capacity Factor)

<u>Annual Costs</u>	<u>Ownership</u>	
	<u>Utility</u>	<u>Industrial</u>
Non-Depreciating Capital	\$ 80,000	\$ 80,000
Depreciating Capital	75,689,000	126,148,000
Operation and Maintenance	2,251,000	2,251,000
Power	<u>153,958,000</u>	<u>236,174,000</u>
Total Annual Cost	\$231,978,000	\$364,653,000
Annual Gas Production	2.74 x 10 <sup>9</sup> std m <sup>3</sup> (10.24 x 10 <sup>10</sup> SCF)	2.74 x 10 <sup>9</sup> std m <sup>3</sup> (10.24 x 10 <sup>10</sup> SCF)
Production Cost	8.47¢/std m <sup>3</sup> (\$2.27/MSCF) \$6.62/GJ (\$6.98/10 <sup>6</sup> Btu)	13.3¢/std m <sup>3</sup> (\$3.56/MSCF) \$10.39/GJ (\$10.95/10 <sup>6</sup> Btu)



case calculation, it is assumed that power costs are 1.28¢/kwh, the capacity factor is 80 percent, and utility ownership prevails.

Figure 4.2.5 shows the effect on hydrogen production cost of variations in the cost of power, for both utility and industrial ownership of the electrolysis plant, with the capacity factor remaining at 80 percent as in the base case. The effect on the production cost of hydrogen, if the oxygen was sold instead of vented, is shown for one assumed value of the oxygen.

Tables 4.2.16 and 4.2.17 indicate the manner in which the capacity factor affects the production costs of both electric power, in the dedicated power station, and hydrogen from the electrolysis plant. In these tables, all of the cost assumptions are the same as the base case with only the capacity factor allowed to vary within a range of 40 to 90 percent. As can be seen, the cost of capital remains constant regardless of how the plant is operated. Operation and maintenance costs are divided into two parts, i.e., fixed and variable. The fixed costs are independent of the plant performance and accrue whether or not the plant is operated. The variable costs are a direct function of the plant operation. Nuclear fuel costs in the power station also have fixed and variable components.

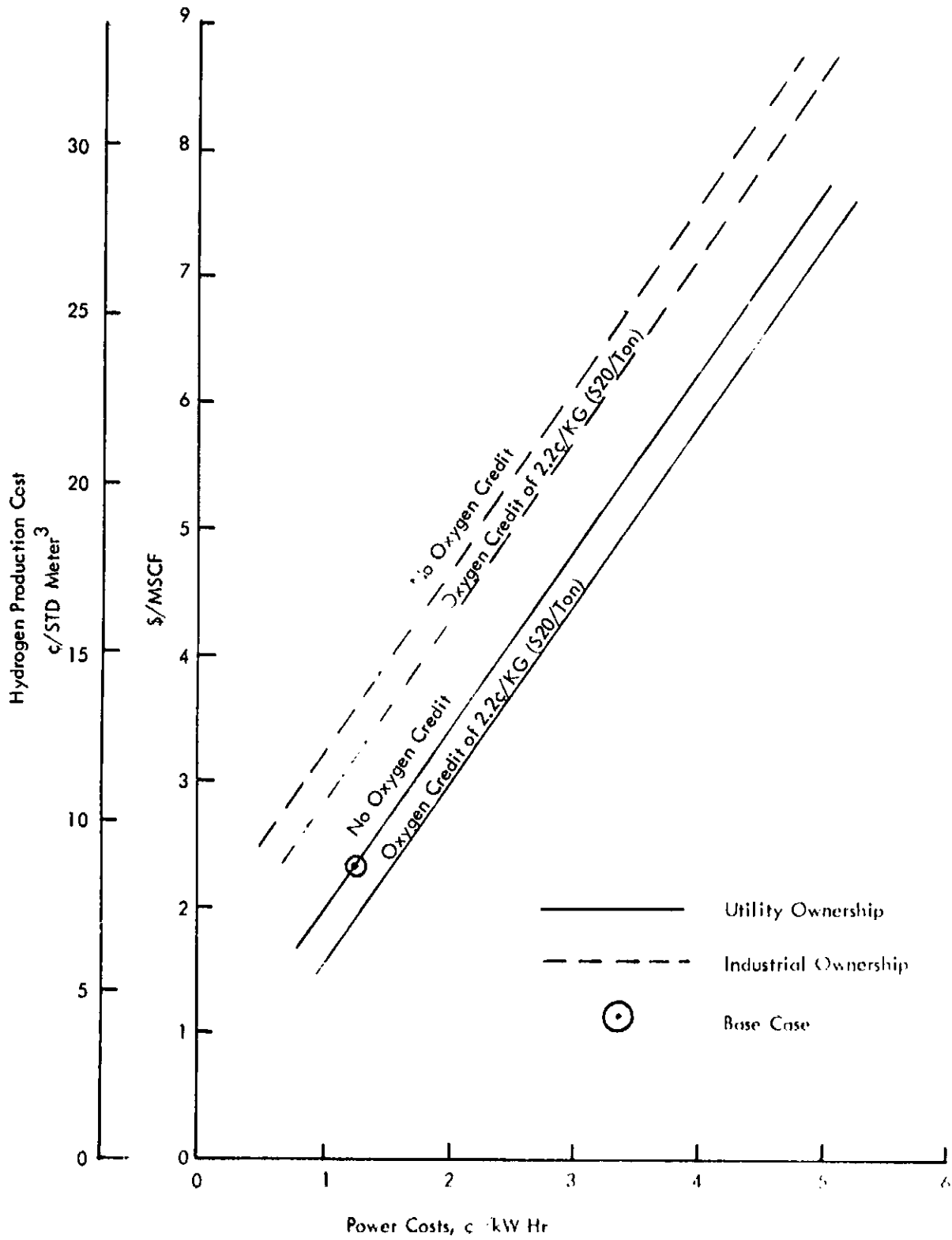


Figure 4.2.5 Water Electrolysis Hydrogen Cost Versus Power Cost

TABLE 4.2.16

## NUCLEAR POWERPLANT

## SENSITIVITY OF POWER COST TO CAPACITY FACTOR

(Base Case Cost Assumptions)

(1720 MWe Capability)

Item	Capacity Factor		
	40%	60%	80%
Capital Cost	\$123,324,000	\$123,324,000	\$123,324,000
Fixed O & M	4,258,000	4,258,000	4,258,000
Variable O & M	546,000	819,000	1,092,000
Fixed Fuel Costs	7,585,000	7,585,000	7,585,000
Variable Fuel Costs	8,850,000	13,274,000	17,699,000
Total Annual Cost	\$144,563,000	\$149,260,000	\$153,958,000
Annual Power Production	0.6 x 10 <sup>10</sup> kwh	0.9 x 10 <sup>10</sup> kwh	1.20 x 10 <sup>10</sup> kwh
Power Cost	2.41¢/kwh	1.66¢/kwh	1.28¢/kwh
			1.36 x 10 <sup>10</sup> kwh
			1.15¢/kwh

TABLE 4.2.17

## WATER ELECTROLYSIS

SENSITIVITY OF H<sub>2</sub> PRODUCTION COST TO CAPACITY FACTOR

(Base Case Cost Assumptions)

	<u>Capacity Factor</u>		
	<u>40%</u>	<u>60%</u>	<u>80%</u>
Capital Cost			
Fixed O & M	\$ 75,769,000	\$ 75,769,000	\$ 75,769,000
Variable O & M	1,840,000	1,840,000	1,840,000
Power	206,000	308,000	411,000
	<u>144,563,000</u>	<u>149,260,000</u>	<u>153,958,000</u>
Total Annual Cost	\$222,378,000	\$227,177,000	\$231,978,000
Annual Gas Production	1.37 x 10 <sup>9</sup> std m <sup>3</sup>	2.06 x 10 <sup>9</sup> std m <sup>3</sup>	2.74 x 10 <sup>9</sup> std m <sup>3</sup>
	(5.12 x 10 <sup>10</sup> SCF)	(7.68 x 10 <sup>10</sup> SCF)	(10.24 x 10 <sup>10</sup> SCF)
Production Cost	16.2¢/std m <sup>3</sup>	11.0¢/std m <sup>3</sup>	8.47¢/std m <sup>3</sup>
	(\$4.34/MSCF)	(\$2.96/MSCF)	(\$2.27/MSCF)
			3.08 x 10 <sup>9</sup> std m <sup>3</sup>
			(11.52 x 10 <sup>10</sup> SCF)
			7.61¢/std m <sup>3</sup>
			(\$2.03/MSCF)

## 4.3 BI-GAS COAL GASIFICATION

### 4.3.1 General

The Bi-Gas coal gasification process is a developing two-stage pressurized gasifier system which represents new technology that could be available in the future for the production of hydrogen from coal. The Bi-Gas gasifier development is being sponsored by Bituminous Coal Research, Inc., American Gas Association, and ERDA.

The work thus far on the Bi-Gas process has been aimed toward the production of high Btu synthetic natural gas e.g., a product gas containing a large fraction of methane. As discussed in Section 4.3.2, this development has progressed to the pilot plant stage. The pilot plant will serve to verify the performance of the two stage gasifier. Testing should demonstrate that a high pressure, 1200 K (1700°F) synthesis gas can indeed be produced and that design and calculational models used heretofore for the gasifier are adequate. Several other aspects of the process are in the development stage and will be evaluated during testing of the pilot plant. These areas include coal feeding, slag removal, char separation, CO shifting, acid gas removal and methanation. Most of the above process items are germane if the process were to be tailored to produce hydrogen. In addition, as a hydrogen producing plant, development of the feedback portion of the process would be required to verify the feasibility of that portion of the process. This would include the steps of cryogenic separation of the methane and hydrogen, with subsequent expansion of the methane to lower pressure, steam/methane reforming, repressurization of the reformed product stream and feedback of this stream into the CO shift converter.

### 4.3.2 The Bi-Gas Process (Reference 34)

The heart of the Bi-Gas process is the two-stage gasifier which uses coal in entrained flow. Fresh pulverized coal is introduced into the upper section (Stage 2) of the gasifier at pressures in the range of 7080 to 10130 kPa (70 to 100 atm), as shown in Figure 4.3.1. Here, the coal comes in contact with a rising stream of hot synthesis gas produced in the lower section (Stage 1) and is partially converted into methane and more synthesis gas.

The residual char entrained in the raw product gas is swept upward and out of the gasifier. The char is separated from the product gas stream and recycled to the lower section (Stage 1) of the gasifier.

In the lower section, the char is completely gasified under slagging conditions with oxygen and steam, producing both the synthesis gas and the heat required in the upper section (Stage 2) for the partial gasification of the fresh coal.

The raw product gas from Stage 2 is purified by removal of hydrogen sulfide and carbon dioxide and processed to the final product in downstream steps.

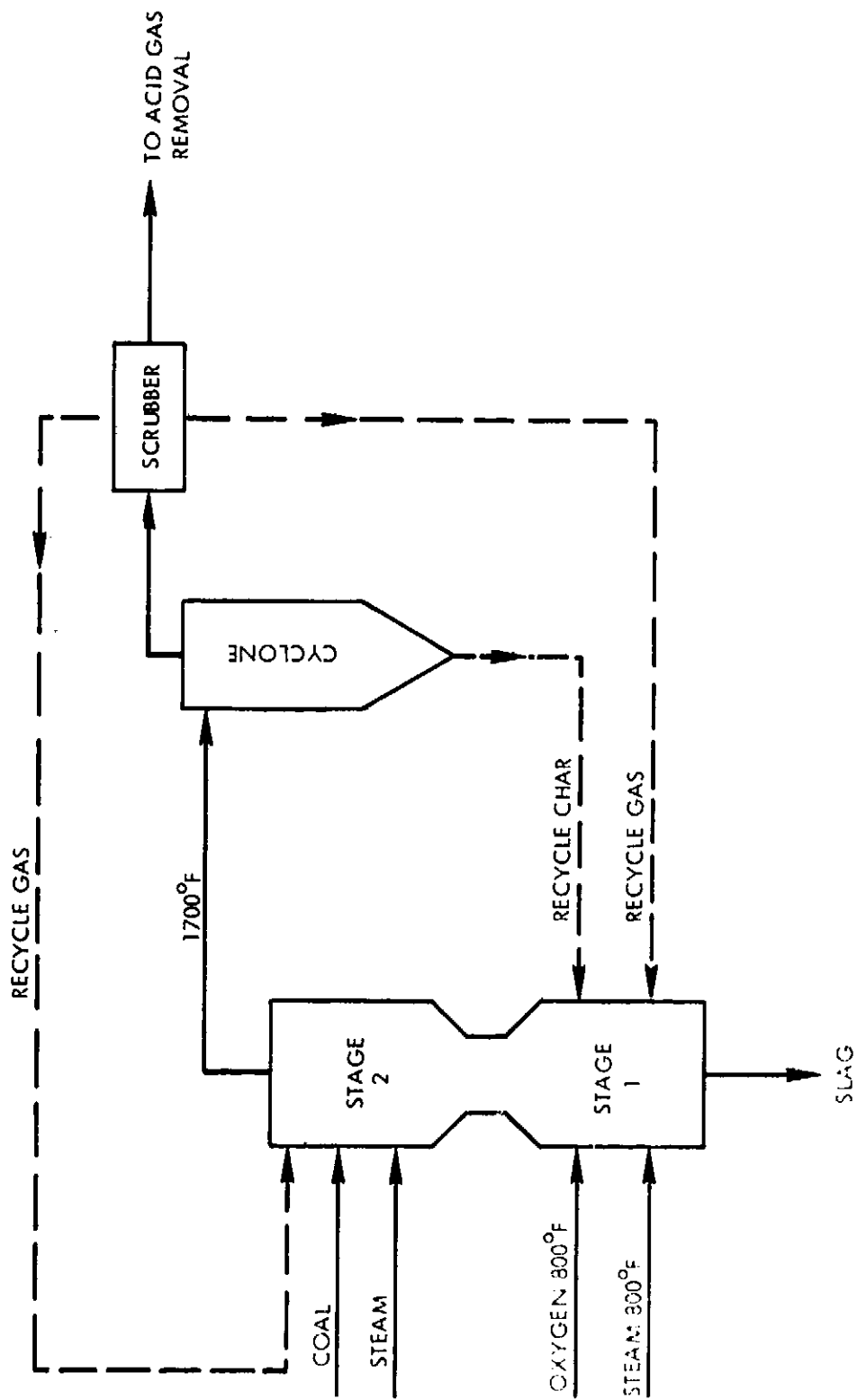


Figure 4.3.1 Bi-Gas Gasification Two Stage Gasifier

The principal objective of the current Bi-Gas research and development program is the production of high-Btu pipeline gas from coal. The initial phase of the program was a world-wide survey of available and proposed coal gasification processes. This survey resulted in a summary of these processes and in the conceptual design of the two-stage, entrained super-pressure, oxygen-blown system for producing high-Btu pipeline gas from coal.

Development work on Bi-Gas has proceeded from batch-type experiments in rocking autoclaves, through continuous flow experiments in a 2.27 kg (5-pound) per hour external heated reactor, to operation of a 45.4 kg (100-pound) per hour internally-fired, Stage 2, process and equipment development unit (PEDU). Using North Dakota lignite, Wyoming subbituminous coal, and Pennsylvania high volatile bituminous coal, the research has confirmed the basic assumption that high yields of methane could be obtained from coal at elevated temperatures and pressures. The essential conclusion of the experiments was that for residence times longer than a fraction of a second, methane yields depended upon coal rank and upon processing conditions such as temperature and hydrogen partial pressure.

With the completion of the Stage 2 PEDU test program, the correlations obtained were used for planning and designing a larger-scale, fully integrated 4536 kg/hr (5-ton per hour) gasification pilot plant at Homer City, Pennsylvania. A bid package for the design of a pilot plant was completed in 1971. Bids for the detailed engineering and construction of the pilot plant were received and the construction contract was awarded in July 1972. Completion of construction of the pilot plant is scheduled for 1975. The overall objective of the pilot plant is to provide sufficient design data for construction of a commercial plant.

The design of the pilot plant represents, to a great extent, the expected design considerations of a commercially sized plant. The description of the pilot plant, below, therefore is applicable to the full scale hydrogen generation process discussed in Section 4.3.3.

Coal, 1-1/2 inch x 0 size, will be received into the plant by both rail and truck. The unloading, conveying and storage equipment is conventional except that the bulk of the storage will be stockpiled. Reclaiming will be accomplished using front-end loaders.

Coal preparation consists only of size reduction. The pilot plant will use coal pulverized to approximately 70 percent minus 200-mesh. However, the pulverizing system is designed with the flexibility to vary both particle size and particle size distribution.

The pulverized coal discharges into a gravity thickener where the solids are concentrated. The solids laden flow from the thickener is fed to a solid bowl type centrifuge where the solids are concentrated into a cake containing 50 percent to 65 percent solids. The cake is then slurried to the consistency used in the process. Flux, if needed for changing slagging characteristics, is added to the slurry at the blend tank. A constantly recirculating slurry stream provides suction volume to the high pressure slurry pumps.

The high pressure slurry feeding system uses feed pumps of the reciprocating type equipped with variable speed drives to feed a high pressure spray drying system. After passing through a shell and tube preheater, the slurry (containing as much as 60 percent solids) is atomized through a spray nozzle. The spray is contacted with a hot inert recycle gas for nearly instant vaporization of the surface water. Leaving the spray dryer, the water vapor-inert gas stream conveys the coal to a cyclone elevated for gravity feed into the gasifier. It is expected that much of the inherent moisture will be removed during the travel. The water vapor-inert gas stream leaving the coal cyclone is water washed to provide both cooling and cleaning before recompression and reheating. A continuously circulating water stream is air-cooled to remove sensible as well as latent heat of water condensation. The condensed water is depressured and returned for reuse in grinding and slurring. Reheat is provided by an indirect fired heater.

The Bi-Gas gasifier has three defined sections; Stage II, Stage I, and the Quench, separated by formed restrictions. The gasifier is a water cooled tube design. The tubes protect both the outer shell of stages one and two, and the inner annulus of stage one from overheating. Many facets of this gasifier design were tested by BCR in a full-scale cold model. Major emphasis was placed on determining the effects of nozzle position and orientation on gasifier operation, particularly with regard to Stage 2 mixing patterns and to slag deposition in Stage 1. All nozzle and burner orientations and locations, as well as throat diameters and volumes for both Stages 1 and 2, were specified by BCR as a result of information developed during the Stage 2 PEDU and the cold model programs. During the model tests, it was also demonstrated that slag carryover into Stage 2, should it occur, can be minimized in either of two ways: by installing vanes in the top of Stage 1 or by admitting some Stage 2 steam at the throat which divides the two stages. Provision for steam injection at the throat has been made.

The gasifier uses pulverized coal in entrained flow. Coal from the cyclone in the slurry feeding system is fluidized by recycle gas and conveyed as a dense phase through two injector nozzles. Steam is also introduced through a separate annulus in the injector. The two streams combine at the tip and join the rising hot synthesis gas from Stage 1. The mixing temperature of about 1476 K (2200°F) is rapidly attained; thus converting the coal to methane, synthesis gas, and char. This raw gas and char leave the gasifier at about 1200 K (1700°F), and are quenched to 750 K (800°F) by atomized water before separation in a char cyclone. The cyclone is elevated in the structure to provide a solids standpipe. However, because char has a density of only 112 to 160 kg/m<sup>3</sup> (7 to 10 pounds per cubic foot), an extremely long standpipe would be required to overcome the 69 to 103 kPa (10 to 15 psi) pressure differential necessary to feed into the first stage. To overcome this pressure differential, a steam eductor is employed using a portion of the steam needed for reaction. The steam and char enter the gasifier reactor through three injection nozzles arranged tangentially to produce a swirl. Oxygen is fed through a separate annulus in the injector and combines with the steam and char as it leaves the injector tip. The mixing temperature of 1755 to 1922 K (2700 to 3000°F) is very rapidly attained to gasify the char completely under slagging conditions. The synthesis gas produced along with any unreacted char and



perhaps some entrained slag pass through the throat into the second stage. As the Stage 1 synthesis gas passes through the throat it is partially quenched with steam to solidify any entrained molten slag and to keep it from touching the walls of Stage 2.

The pilot plant gasifier is designed for coal feed rates up to 4536 kg/hr (5 tons per hour) and a maximum operating pressure of 10340 kPa (1500 psi). Speed of the coal particle entering Stage 2 will range from 6.1 to 9.1 m/s (20 to 30 fps). The resultant char particles will slow down to about 0.5 to 0.76 m/s (1.5 to 2.5 fps) in their passage through Stage 2. Typical residence times will be 2 seconds in Stage 1 and 8 to 10 seconds in Stage 2. The reactor cooling system is a subcooled, forced circulation water system. It is equalized with the process system pressure and maintained at a temperature above the dew point of the process gases to avoid condensation. It is extensively instrumented to enable early detection of any abnormality. The system is powered by both electricity and steam and automated to make it highly reliable in such critical service.

In the slag removal system, molten slag is deposited on the walls of Stage 1 and flows out the slag tap opening in the bottom conical section. Two burner devices have been added to assist in keeping the slag molten and free flowing. The slag heating burners direct a natural gas-oxygen flame on the top side of the cone and a pencil-like flame from the slag tap burner is directed up through the slag tap opening. A slag breaker is provided to knock off any stalactite which may form.

The molten slag drops into a reservoir of water in the bottom of the gasifier for rapid quenching, causing the slag to shatter into small pieces.

The walls of the quench section are continuously sprayed to provide cooling and also to wash down any slag splatter which may occur. The slag falls through the water and exits the gasifier through either one of two bottom openings, assisted by the recirculating water. Two such lockhoppers are installed to provide continuous removal while one is being depressured and emptied. Provision is also made for removal of floating char should any accumulate on the surface of the slag quench water. The recirculating water passes through the lockhopper, then is repumped through a cooler and returned to the quench section. Fresh water is continuously added and withdrawn to reduce the concentration of salts and fines. The slag slurry removed from the lockhoppers is pumped to a settling pond. The clarified water from the settling pond is reused for filling the slag lockhoppers and for dust and fume scrubbing as needed. Solids are manually removed from the settling pond where necessary.

During cleanup of the raw gas, the gas leaving the char cyclone passes through a water wash column where the gas is further cooled and the dust is removed. Moisture is needed for the downstream shift conversion; therefore, the wash column will be operated at conditions to maintain only the required moisture while the surplus is condensed. The water is cooled by recirculation through an aerial cooler. Fresh water is added as needed to remove solids and salts from the system. Purged water is flashed at low pressure and sent to

disposal. A separate section is provided in the upper part of the washer for possible chemical wash if needed. Also, provisions are made for removal of floating char and oil, if needed.

The remainder of the pilot plant process steps, with the exception of methanation, are existing commercial operations. The same, or different, process steps can be used in the full scale plants depending on the final products as desired.

#### 4.3.3 Hydrogen Production Plant

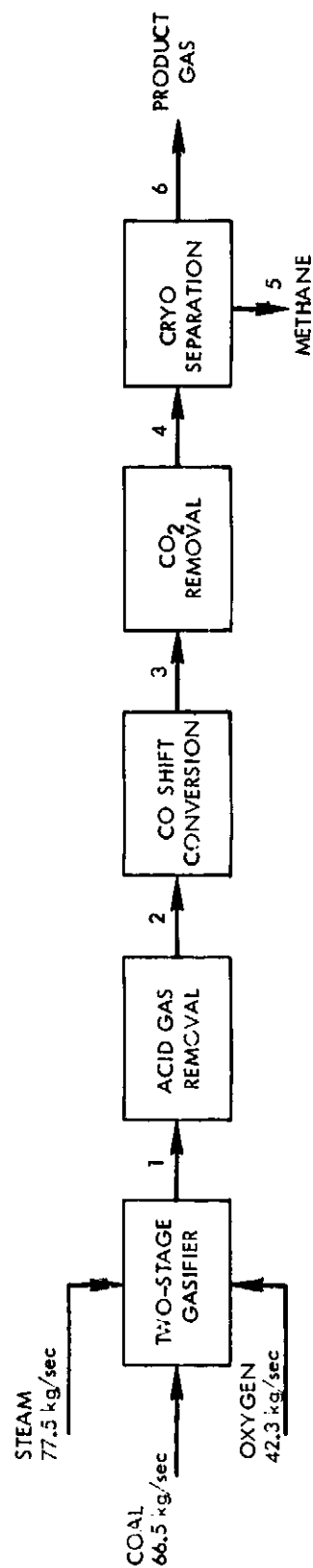
If used for hydrogen production primarily, the Bi-Gas process must undergo some modifications from its original purpose. The Bi-Gas process is being developed primarily for production of high Btu pipeline quality gas with ~95% methane (volume composition) in the final product stream. However prior to methanation, the gas volume composition is ~60% hydrogen, and 20% methane and 20% carbon monoxide. Removing the methanation step therefore does provide a reasonably high yield of hydrogen which can be further increased by appropriate conversion, e.g., steam reforming of the methane.

For purposes of this study of hydrogen production processes, it is beyond the scope of the program to perform major detailed modifications of the Bi-Gas process so as to optimize the process for hydrogen output. Nevertheless, two options for obtaining a high purity hydrogen product stream were scoped for evaluation. An overall process diagram for one option is shown in Figure 4.3.2, where the hydrogen and methane are separated via cryogenic separation. This option, sized for  $9.65 \times 10^6$  std  $m^3$ /day ( $360 \times 10^6$  SCFD) of hydrogen, requires a coal feed of 66.5 kg/s (6335 tons/day) into the gasifier. With 2.28 std  $m^3$ /day ( $85 \times 10^6$  SCFD) of methane also being produced, this option in effect provides a dual purpose plant.

The overall process diagrams for the second option is shown in Figure 4.3.3. In this case the methane is taken from the cryogenic separator and reformed with steam to create more hydrogen. The reformed product gas is then fed back to the CO shift converter and mixed with the main stream gas into the shift stage. This option, with hydrogen as its sole product, requires ~27% less feedstock to the gasifier than the dual purpose option (compared at the same hydrogen output). This option, with reforming of methane, has been used as the reference configuration in evaluation of Bi-Gas for hydrogen production.

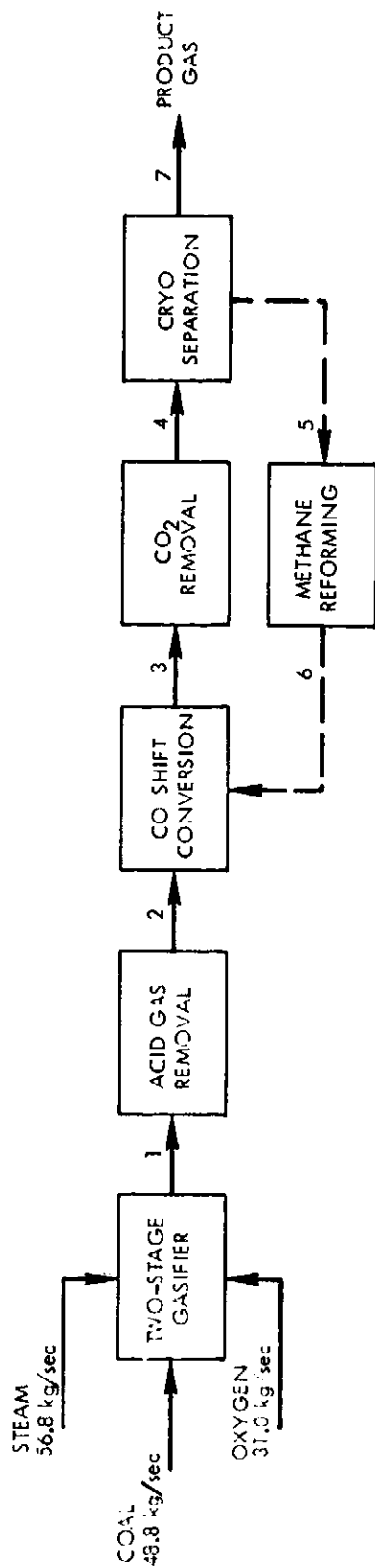
Table 4.3.1 summarizes the estimated operating characteristics of the reference process. It should be noted that only about 60% of the total coal required for the plant is used as feedstock for the gasifier with the remainder used to produce steam for the various process units and auxiliary equipment.

The heart of the Bi-Gas process is the two-stage gasifier. Pulverized coal is introduced into the upper section (Stage 2) at 7090 to 10130 kPa (70 to 100 atmospheres). Here the coal comes in contact with a rising stream of hot synthesis gas that has been produced in the lower section (Stage 1). In Stage 2, the coal is partially converted to methane



STREAM NO.	1	2	3	4	5	6
VOLUME FLOW - std m <sup>3</sup> /day	17.4 x 10 <sup>6</sup>	16.3 x 10 <sup>6</sup>	32.1 x 10 <sup>6</sup>	11.3 x 10 <sup>6</sup>	2.28 x 10 <sup>6</sup>	9.65 x 10 <sup>6</sup>
VOLUME FRACTION - %						
H <sub>2</sub>	24.2	28.6	27.3	77.4	--	99.3
CO	22.1	26.1	0.6	1.6	--	TRACE
CO <sub>2</sub>	16.2	--	12.7	0.1	--	--
CH <sub>4</sub>	11.8	14.0	7.1	20.1	100	--
N <sub>2</sub>	0.5	0.6	0.3	0.8	--	0.7
H <sub>2</sub> S	0.6	--	--	--	--	--
H <sub>2</sub> O	24.6	30.7	51.9	--	--	--

Figure 4.3.2 Bi-Gas Coal Gasification - Overall Process Diagram



	1	2	3	4	5	6	7
STREAM NO.							
VOLUME FLOW - std m <sup>3</sup> /day	12.8 x 10 <sup>6</sup>	10.8 x 10 <sup>6</sup>	28.48 x 10 <sup>6</sup>	12.03 x 10 <sup>6</sup>	2.36 x 10 <sup>6</sup>	8.92 x 10 <sup>6</sup>	9.65 x 10 <sup>6</sup>
VOLUME FRACTION - %							
H <sub>2</sub>	24.2	28.6	33.6	79.8	--	37.1	99.3
CO	22.1	26.1	--	--	--	4.0	TRACE
CO <sub>2</sub>	16.2	--	13.1	0.1	--	6.2	--
CH <sub>4</sub>	11.8	14.0	8.3	19.6	100	9.6	--
N <sub>2</sub>	0.5	0.6	0.2	0.5	--	--	0.7
H <sub>2</sub> S	0.6	--	--	--	--	--	--
H <sub>2</sub> O	24.6	30.7	44.8	--	--	43.0	--

Figure 4.3.3 Bi-Gas Coal Gasification - Overall Process Diagram

TABLE 4.3.1

BI-GAS GASIFICATION  
OPERATING CHARACTERISTICS

Hydrogen Output	$9.65 \times 10^6$ std m <sup>3</sup> /day ( $360 \times 10^6$ SCFD)
Coal Feed to Gasifier	176,000 kg/hr (184 Ton/hr)
Total Plant Coal Consumption	301,200 kg/hr (332 Ton/hr)
Gasifier Output	
Temperature	1200 K (1700°F)
Pressure	6895 kPa (1000 psi)
Flow Rate - Tons/Hour	491,700 Kg/hr (542 Ton/hr)
Overall Process Efficiency	46%

and more synthesis gas. The raw gas output from Stage 2 including entrained residual char is sent to waste heat boilers and char cyclone where the char is separated from the gas and recycled to Stage 1 of the gasifier. Also a portion of the synthesis gas is recycled to both stages of the gasifier.

Figure 4.3.4 displays the mass and volumetric process flow rates for major stages of the process. The coal breakdown shown in stream 1 is based on Pittsburgh seam coal. Once the high temperature, high pressure synthesis gas has been produced (stream 4), it is cooled by waste heat boilers (not shown) before going to the acid gas removal stage. In this stage, effectively all of the sulfur is removed via an amine system using caustic fluid circuits. In effect, the acid gas removal, CO shift converter and CO<sub>2</sub> removal stages function in a similar manner to those comparable stages described for the Koppers-Totzek process in Section 4.4.3. The major points of difference within these units between the Bi-Gas and K-T plants is the composition of the synthesis gas being treated. Because of the relatively high methane content of the gas after CO<sub>2</sub> removal, the use of the cryogenic separation and methane cracking units was indicated for Bi-Gas to enhance hydrogen production.

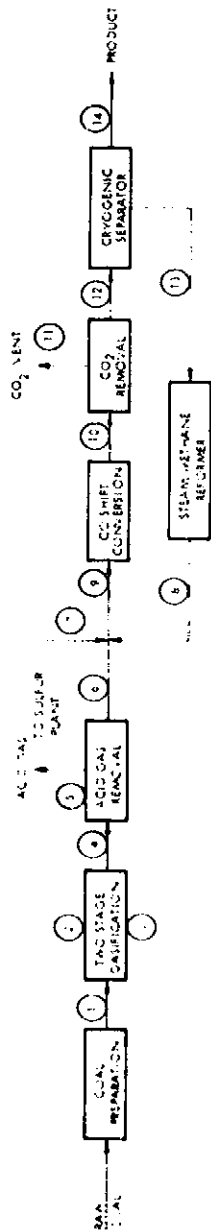
Before separation of the methane, the product stream is expanded to drop its pressure from 709 kPa (70 atm) to 3545 kPa (35 atm). Liquefaction of the methane then occurs within the cryogenic separator at ~165K. The separated methane is then sent to the steam-methane reformer with ~25% of the total diverted as fuel to fire the reformer. The methane steam reaction within the reformer produces a product gas with the composition shown in stream 8 of Figure 4.3.4. Following condensation of the steam and removal of the condensation, the hydrogen rich reformer product is compressed back to 7090 kPa (70 atm,) and fed back to the CO shift converter unit along with the main stream synthesis gas from the acid gas removal unit.

#### 4.3.4 Plant Performance Characteristics

The performance of the plant can be experienced in several different ways. The paragraphs below summarize the performance in terms of resource consumption, process outflows, and overall thermal efficiency.

##### 4.3.4.1 Resource Consumption

For purposes of evaluation, the only resources considered are those associated with the operation of the plant, and not with the manufacture or construction of the facility. The resources are categorized into coal, consumptive water use, electricity, and chemicals catalysts. Included in this last item is limestone consumption for the slurry flue gas clean-up system used with the coal fired steam boilers in the plant. Table 4.3.2 summarizes the annual consumption of these materials. It should be noted that, for purposes of conservatism, it was assumed that all catalysts would be replaced annually. The resource impact of the electric power consumed would be a function of the mix of power plants in the utility system, and therefore not specified in more detail in the table.



GENERAL PROCESS BALANCE

STREAM NUMBER	STREAM NAME	4		5		6		7		8		9		10		11		12		13		14		15		
		Wt. %	Flow	Wt. %	Flow	Wt. %	Flow	Wt. %	Flow	Wt. %	Flow	Wt. %	Flow	Wt. %	Flow	Wt. %	Flow	Wt. %	Flow	Wt. %	Flow	Wt. %	Flow	Wt. %	Flow	
1	RAW GAS																									
2	COAL PREPARATION																									
3	TWO STAGE GASIFICATION																									
4	ACID GAS REMOVAL																									
5	ACID GAS REMOVAL																									
6	ACID GAS REMOVAL																									
7	ACID GAS REMOVAL																									
8	ACID GAS REMOVAL																									
9	ACID GAS REMOVAL																									
10	ACID GAS REMOVAL																									
11	ACID GAS REMOVAL																									
12	ACID GAS REMOVAL																									
13	ACID GAS REMOVAL																									
14	ACID GAS REMOVAL																									
15	STEAM METHANE REFORMER																									
TOTAL																										

Figure 4.3.4. Hydrogen Production Using Bi-Gas Coal Gasification

TABLE 4.3.2

BI-GAS GASIFICATION ANNUAL RESOURCE CONSUMPTION  
(80% Capacity Factor)

Coal	$2.13 \times 10^9$ Kg ( $4.7 \times 10^9$ LB)
Water	$1.95 \times 10^{10}$ Kg ( $4.3 \times 10^{10}$ LB)
Electricity	$7.0 \times 10^8$ KWH
Catalysts/Chemicals	$1.36 \times 10^8$ Kg ( $3.0 \times 10^8$ LB)

4.3.4.2 Process Outflows

The products of the process operations, in addition to the hydrogen stream, include a myriad of other flows. The process outflows, on an annual basis, are shown in Table 4.3.3.

TABLE 4.3.3

BI-GAS GASIFICATION  
ANNUAL PROCESS OUTFLOWS  
(80% CAPACITY FACTOR)

Product Hydrogen Stream	$2.82 \times 10^9$ std m <sup>3</sup> ( $1.05 \times 10^{11}$ SCF)
Waste streams	
CO <sub>2</sub>	$1.1 \times 10^9$ std m <sup>3</sup> ( $4.1 \times 10^{10}$ SCF)
Solids	$4.99 \times 10^8$ kg ( $1.1 \times 10^9$ LB)

4.3.4.3 Process Thermal Efficiency

Thermal efficiency can be expressed in many ways. In Table 4.3.4, it is defined as the higher heating value of the product gas divided by the total heat inputs to the hydrogen generation plant. This includes, of course, not only the energy content of the coal being gasified, but also the energy content of the coal and electric power (at an assumed thermal efficiency of 36%) required for the oxygen plant and other steam and electric power requirements.



TABLE 4.3.4

BI-GAS GASIFICATION  
OVERALL PROCESS EFFICIENCY

<u>Heat Inputs</u>	
Coal to Gasifiers	5904 GJ/hr ( $5.6 \times 10^9$ BTU/hr)
Other Heat Inputs (coal for steaming, electric power, etc)	5271 GJ/hr ( $5.0 \times 10^9$ BTU/hr)
TOTAL Heat Input	11,175 GJ/hr ( $10.6 \times 10^9$ BTU/hr)
<u>Heat Output</u>	
Product Gas Heating Value	$4.02 \times 10^5$ std m <sup>3</sup> /hr ( $15 \times 10^6$ SCF/hr) 12.71 MJ/std m <sup>3</sup> (323 Btu/SCF)
TOTAL Heat Output	5108 GJ/hr ( $4.845 \times 10^9$ BTU/hr)

Overall Efficiency

$$\frac{5108 \text{ GJ/hr} \times 100}{11,175 \text{ GJ/hr}} = 45.7\%$$

4.3.5 Economics

As part of the overall evaluation of the Bi-Gas process for hydrogen production, estimates were made of the economics of the  $9.65 \times 10^6$  std m<sup>3</sup>/day ( $360 \times 10^6$  SCFD) hydrogen plant. In preparing the cost estimates, close coordination was maintained with efforts on the other coal gasification process, Koppers-Totzek, to ensure consistency of approach and continuity of ground rules and assumptions. In determining the overall costs, estimates were made of the capital, operation and maintenance, and fuel costs for the facility in the general format used in reporting nuclear power plant costs, as defined in NUS-531 (Reference 32). The effects on the production costs of different capacity factors, fuel costs, and type of ownership were also considered.

4.3.5.1 Capital Costs

The capital costs estimate is based on preliminary sizing of most of the major plant equipment and determining appropriate costs for that equipment. Factors, based on experience with these types of systems, were used to account for the costs of installation, piping, valves, instrumentation, structures, and miscellaneous equipment. Indirect costs were also estimated by applying factors in the manner described below.

The hydrogen production plant is estimated to require a direct cost investment, in mid-1974 dollars, of \$230,308,000, as shown in Table 4.3.5. The direct cost is presented according to a code of accounts that divides systems among on-sites and off sites, with the former consisting of closely related mainline processing steps and the latter consisting of support and service systems and facilities.

The total plant investment, shown in Table 4.3.6, includes the direct costs plus contingencies, indirect costs, and interest during construction. For the purpose of evaluation, land and land rights are shown separately from other direct costs since it is a non-depreciating asset.

Special materials comprise the initial supply of chemicals, catalysts, lubricants and other materials needed for operation of the plant. A contingency of 15 percent is applied to the estimated cost of the special materials and the direct cost of the physical plant.

Indirect costs are expense items of a general nature which apply to the overall project of building an operable plant, rather than to one of the direct costs. These costs, except for interest during construction, have not been estimated in detail, but calculated as a percentage of the direct costs based on the procedure defined in NUS-531 and updated by ERDA in 1974 for use in the economic analysis reported in Reference 1.

Construction facilities, equipment, and services include general costs associated with the plant construction, such as field offices, warehouses, temporary power and utility lines, cost or rental of construction equipment and supplies, purchase of electric power, water, and other utilities, security guards, training programs for the labor force, inspection and testing of construction materials, site cleanup, insurance, and the like.

Engineering services include items such as preliminary investigations; site selection; air and water environmental studies; subsurface investigations; preparation of specifications and evaluation of proposals for major equipment packages, preparation of preliminary and final design documents, design reviews, procurement, inspection, and expediting of materials and equipment; preparation of pre-operational test and plant startup procedures; assistance in securing plant permits; management and direction of construction activities, including selection of subcontractors, scheduling, maintaining cost and quality control; on-site procurement and receiving of materials and equipment; field accounting; supervising and pre-operational testing of systems and components; field engineering inspection of construction work to assure compliance with plans and specifications; and preparation of as-built drawings.

Other costs include the owner's property and all-risk insurance, state and local property taxes on the site and improvements during construction, sales taxes on purchased materials and equipment, staff training, plant startup, and the owner's general and administrative (G&A) costs.

TABLE 4.3.5  
BI-GAS GASIFICATION  
DIRECT CAPITAL COSTS  
(JULY 1974 DOLLARS)

<u>Account</u>	<u>Item</u>	<u>Installed Cost</u> <u>(\$ THOUSANDS)</u>
<u>2000</u>	<u>On-Sites</u>	
2100	Coal Preparation	9,381
2200	Coal Gasification	48,283
2300	Acid Gas Removal	7,226
2400	CO Shift	16,534
2500	CO Removal	9,845
2700	Oxygen Plant	23,612
2800	Sulfur Recovery Plant	2,436
2900	Compression	7,785
2950	Cryogenic Separators Unit	21,600
2960	Reformer Unit	21,150
	<u>On-Sites Subtotal</u>	<u>\$ 167,852</u>
<u>1000</u>	<u>Off-Sites</u>	
1100	Cooling Towers	20,140
1200	Makeup and Feedwater	1,085
1300	Effluent Water Treatment	7,073
1410	Coal Storage & Handling	815
1420	Slag Disposal	10,622
1430	Flue Gas Cleanup	4,545
1510	Steam Generating Plants	11,185
1600	Electrical Auxiliary Power	--
1700	General Off-Site Investment	1,000
1710	Land & Land Rights	2,334
1720	Site Improvements & Facilities	734
1730	Administrative Service Building	610
1740	Instrumentation & Plant Air	1,293
1750	Maintenance Facilities	485
1760	Fire Protection	325
1770	Furnishing, Fixtures	--
	<u>Off-Sites Subtotal</u>	<u>\$ 62,456</u>
	<u>Total Direct Capital Cost</u>	<u>\$ 230,308</u>

TABLE 4.3.6  
BI-GAS GASIFICATION  
ESTIMATED CAPITAL COST SUMMARY  
(In Thousands of Dollars)

<u>Non-Depreciating Assets</u>	Cost
Land and Land Rights	\$ 1,000
<u>Depreciating Assets</u>	
Special Materials	3,285
Physical Plant	<u>229,308</u>
Subtotal	232,593
Contingency	<u>34,889</u>
Subtotal	267,482
<u>Indirect Costs</u>	
Construction Facilities, Equipment and Services	\$ 15,247
Engineering Services	\$ 23,271
Other Costs	\$ 7,649
Interest During Construction	<u>\$ 45,861</u>
Subtotal	\$ 92,028
Total Depreciating Assets	\$ 359,510
Total Plant Investment	\$ 360,510

Interest during construction is calculated as simple interest, at an 8 percent annual rate, on the plant investment as it is made. For the purpose of the evaluation, it is assumed that the land is purchased six months prior to the start of the project and that special materials are delivered and paid for nine months prior to plant commercial operation. The remainder of the plant investment is made as design and construction proceeds as shown in Figure 4.3.5. The project schedule includes an initial two year period in which expenditures remain low while engineering proceeds, environmental impact statements are prepared, and permits for construction are solicited.

The total plant investment, including all direct and indirect costs but excluding escalation, is estimated to be \$360,510,000 for the grass roots facility.

#### 4.3.5.2 Operation and Maintenance Costs

The costs of operation and maintenance includes the expense of maintaining a plant staff, consumable supplies and equipment, outside support services, miscellaneous items of cost, and indirect costs of maintaining the plant working capital.

The direct O&M costs are shown in Table 4.3.7. The staff costs are based on a 180 person staffing level at an average cost of \$19,300 per man-year. The costs of chemicals and catalysts are based on their assumed use rate. An allowance has been included for miscellaneous consumables.

Outside support services are taken to embrace all services obtained other than from the normal plant complement during normal working hours. Other requirements for outside support services include such items as off-site disposal of wastes, major equipment overhauls, and consultants to provide various forms of operational support.

Miscellaneous O&M costs include such items as training new staff personnel, requalification of operators, rent (for property, equipment, or facilities which are used or occupied in connection with plant operation), travel, such as to staff conferences at the main office, or to professional society meetings or other conferences, licenses and fees, office supplies, postage, and telephone/telegraph bills, and fuel and upkeep of station vehicles.

The total direct annual operation and maintenance cost of \$9,853,000 includes a 15 percent G&A assessment on all costs.

The indirect O&M costs are shown in Table 4.3.8. These are the costs of maintaining the working capital required for continued operation of the plant and is evaluated at a 10 percent annual charge rate. The working capital is made up of the cash in hand needed to meet the day to day operating expenses plus the value of materials and supplies in inventory. The average net cash required is calculated at 2.7 percent of the direct O&M costs. A two month supply of coal consumables is assumed to be kept in inventory. The coal is valued, for this purpose, at 2.2¢/kg (\$20/ton).

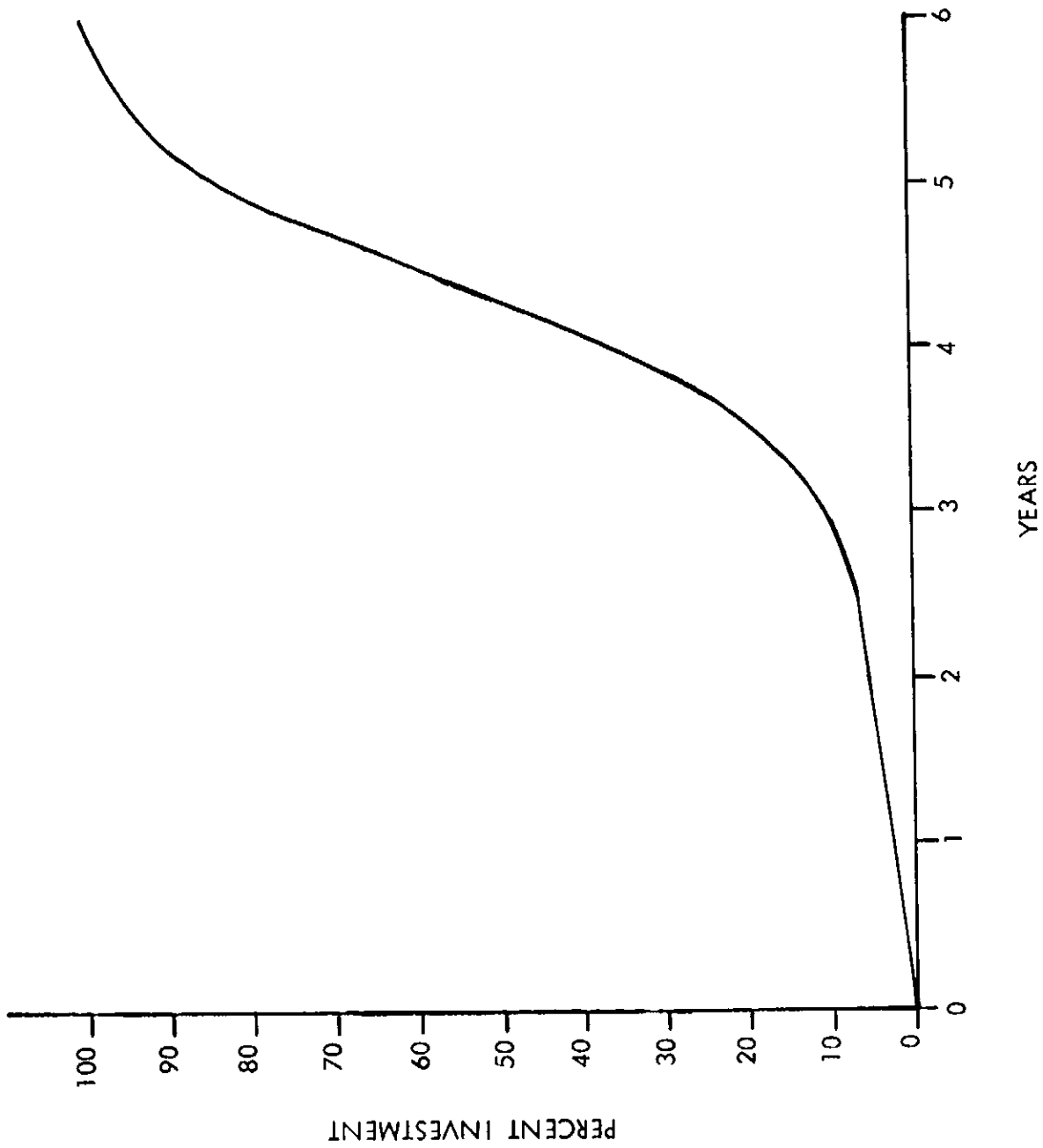


Figure 4.3.5 Coal Gasification - Plant Capital Investment Expenditures Versus Time

TABLE 4.3.7

BI-GAS GASIFICATION

DIRECT ANNUAL O & M COSTS

Staff Payroll	\$ 3,474,000
Consumable Supplies and Equipment	\$ 4,237,000
Outside Support Services	\$ 777,000
Miscellaneous	\$ <u>80,000</u>
Subtotal	\$ 8,568,000
G & A	\$ <u>1,285,000</u>
Total Direct O & M Costs	\$ 9,853,000

TABLE 4.3.8  
BI-GAS GASIFICATION  
INDIRECT OPERATION AND MAINTENANCE COSTS

	<u>Cost</u>
Average Net Cash Required	\$ 266,000
Materials and Supplies in Inventory	
Consumable Supplies and Equipment	\$ 670,000
Coal Storage	\$ <u>11,232,000</u>
Total Working Capital	\$ 12,168,000
Annual Charge Rate	10%
Annual Indirect O & M Cost	\$ 1,216,800

TABLE 4.3.9  
NUCLEAR WATER DECOMPOSITION  
TOTAL ANNUAL O & M COST  
(80% Capacity Factor)

	<u>Cost</u>
Direct O & M Costs	\$ 9,853,000
Indirect O & M Costs	\$ <u>1,217,000</u>
Total	\$ 11,070,000



The total O&M costs, at a plant capacity factor of 80 percent, are shown in Table 4.3.9.

#### 4.3.5.3 Fuel Costs

Fuel costs, as used here, include the purchase of feedstock and energy, i.e., coal and electric power. For the purpose of a base coal calculation, coal, f.o.b. plant site, is allowed to cost 2.2¢/kg (\$20/ton) and electricity, at an industrial customer rate than the utility sites, is costed at 2¢/Kwh.

The plant, operating at an 80 percent capacity factor will consume  $2.11 \times 10^9$  kg/yr ( $2.33 \times 10^6$  Ton/yr) of coal and  $7 \times 10^8$  kwh of electric power, resulting in a total annual "fuel" cost of \$60,590,000.

#### 4.3.5.4 Hydrogen Production Costs

The hydrogen production cost is made up of the contributions of capital, operation and maintenance, and fuel costs. These are normally calculated on an annual basis. The percentage of the plant investment that is charged against production each year is a fraction of the type of plant ownership, i.e., utility or industrial, and the manner in which the owner can do business. As discussed in Section 4.1.2, the annual charge on non-depreciating assets, e.g., land, is 10 percent for either type of ownership while the annual charge on depreciating assets is 15 percent for utility ownership and 25 percent for industrial ownership. Although production costs are calculated on both a utility and industrial basis, it is not realistic to consider that the production of hydrogen, on the scale contemplated and with distribution to remote "users", would be an "industrial" enterprise. It is considered that this sort of production plant would much more readily fit a "regulated utility" type of enterprise - much like today's natural gas and electric utility operations.

The cost of hydrogen production, on both bases, is shown in Table 4.3.10. As can be seen, the cost, which is equivalent to a "gate selling price", is 4.48¢/standard m<sup>3</sup> (\$1.20/MSCF), or \$3.17/GJ (\$3.71/10<sup>6</sup> Btu) on a utility basis. The cost to the ultimate consumer would be this production cost plus the allocated capital and operating costs of transmission and distribution.

#### 4.3.5.5 Sensitivity of Hydrogen Production Costs to Variables

The cost of hydrogen production from any given plant will vary with the cost of fuel, the type of ownership, and the utilization, i.e., capacity factor, of the facility. For the base case calculation, it was assumed that coal costs were 2.2¢/kg (\$20/ton), electricity costs were 2¢/kwh, the capacity factor was 80 percent, and utility ownership prevailed.

TABLE 4.3.10  
 BI-GAS GASIFICATION  
 HYDROGEN PRODUCTION COST COMPARISON  
 (80% Capacity Factor)

<u>Annual Costs</u>	<u>Ownership</u>	
	<u>Utility</u>	<u>Industrial</u>
Non-Depreciating Capital	\$ 100,000	\$ 100,000
Depreciating Capital	53,927,000	89,878,000
Operation and Maintenance	11,070,000	11,070,000
"Fuel"	<u>60,590,000</u>	<u>60,590,000</u>
Total Annual Cost	\$ 125,687,000	\$ 161,638,000
<u>Annual Gas Production</u>	2.82 × 10 <sup>9</sup> std m <sup>3</sup> (1.05 × 10 <sup>11</sup> SCF)	2.82 × 10 <sup>9</sup> std m <sup>3</sup> (1.05 × 10 <sup>11</sup> SCF)
<u>Production Cost</u>	4.46¢/std m <sup>3</sup> (\$1.20/MSCF) \$3.51/GJ (\$3.71/10 <sup>6</sup> Btu)	5.73¢/std m <sup>3</sup> (\$1.54/MSCF) \$4.51/GJ (\$4.76/10 <sup>6</sup> Btu)

Figure 4.3.6 shows the effect on hydrogen production cost of variations in the cost of fuel and electric power for both utility and industrial ownership, with the capacity factor remaining at 80 percent as in the base case.

Table 4.3.11 indicates the manner in which the capacity factor affects the production cost. In this table, all of the cost assumptions are the same as the base case with only the capacity factor allowed to vary within a range of 40 to 90 percent. As can be seen, the cost of capital remains constant regardless of how the plant is operated. Operation and maintenance costs are divided into two parts, i.e., fixed and variable. The fixed costs are independent of the plant performance and accrue whether or not the plant is operated. The variable costs are a direct function of the plant operation.

#### 4.3.6 Alternative Configuration - Dual Purpose Bi-Gas Process

While this study has been based on the reference plant that produces hydrogen as its sole product, no conclusion should be reached to the effect that such a plant would be the optimum use of the Bi-Gas process. For example, the dual-purpose approach, as introduced in Section 4.3.3 and shown in process form in Figure 4.3.2, would produce both hydrogen and methane.

Although detailed analysis of the alternative configuration is beyond the scope of this study, it is instructive to examine the relative economics of this alternative approach. This was done by appropriate adjustments to the economic estimates for the reference plant that were presented in Section 4.3.5. Table 4.3.12 summarizes the estimated production costs of hydrogen and methane for the dual purpose process, based on the same hydrogen production rates in both cases. Comparison of the annual costs in Table 4.3.12 with those for the reference plant, Table 4.3.10, indicates that the dual purpose plant costs would be approximately 5 percent higher, primarily because of the additional fuel used. The annual costs for depreciating capital and operation and maintenance would be less for the dual purpose plant because of the elimination of the methane reforming stage. Elimination of this item, which was more than \$21,000,000 (Table 4.3.5), more than off-set cost increases in other units caused by larger size ratings.

The dual purpose alternative was sized to produce the same hydrogen output as the reference plant, and the methane produced would provide ~40 percent of the total heating value of both methane and hydrogen. For this reason, the production costs for the dual purpose plant, as shown in Table 4.3.12, are significantly less than for the reference (hydrogen only) plant. Therefore, if the Bi-Gas process were to be tailored to be a hydrogen producer, the economics would favor use of methane as a valuable secondary product rather than as a recycled feedstock to enhance hydrogen production.

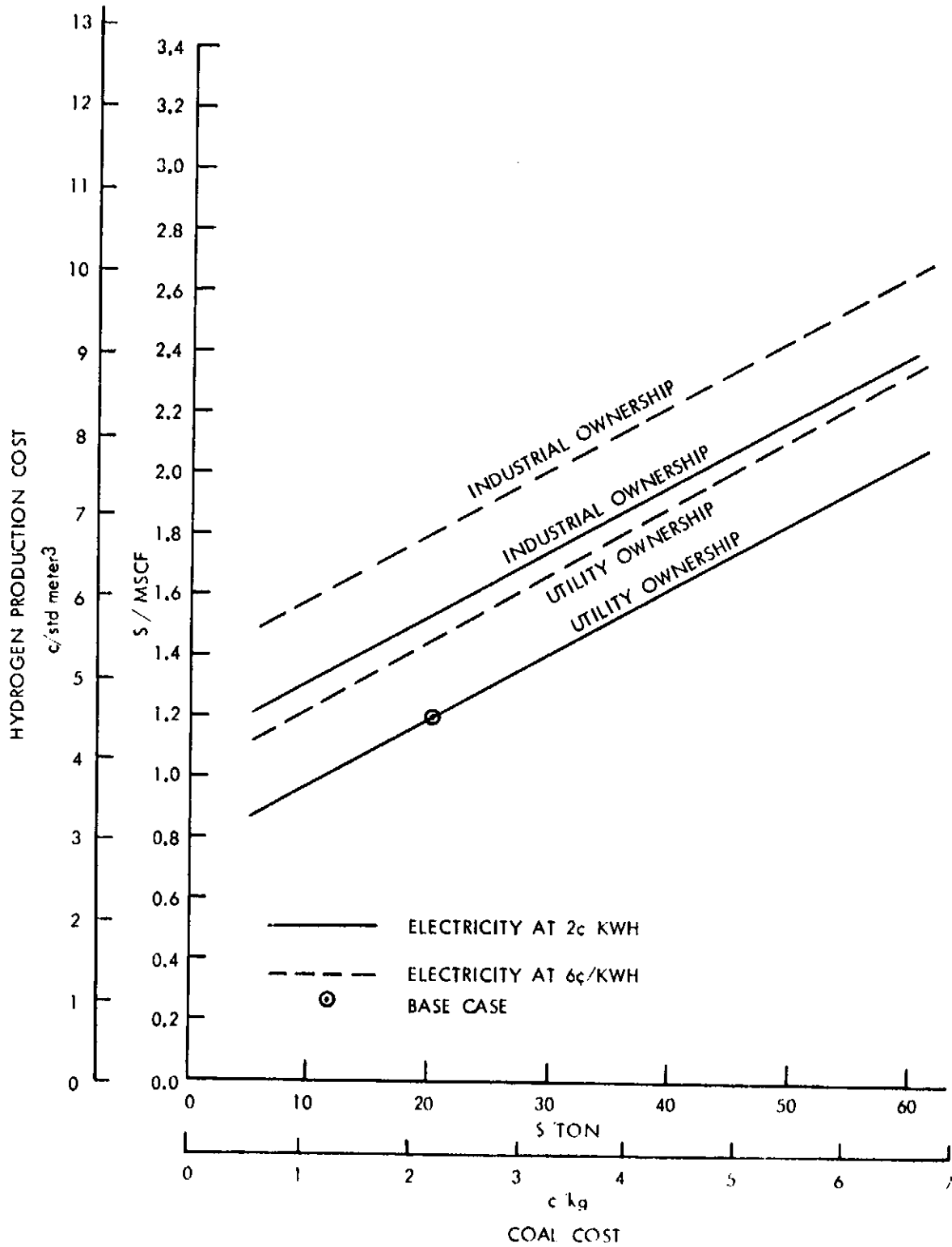


Figure 4.3.6 Bi-Gas Gasification - Hydrogen Cost versus Cost of Coal (80% Capacity Factor)

TABLE 4.3.11

## BI-GAS GASIFICATION

SENSITIVITY OF H<sub>2</sub> PRODUCTION COST TO CAPACITY FACTOR

(Base Case Cost Assumptions)

Item	Capacity Factor		
	40%	60%	80%
Capital Cost	54,027,000	54,027,000	54,027,000
Fixed O & M	5,694,000	5,694,000	5,694,000
Variable O & M	2,688,000	4,032,000	5,376,000
Fuel Costs	<u>30,295,000</u>	<u>45,443,000</u>	<u>60,590,000</u>
Total Annual Cost	92,704,000	109,196,000	125,687,000
Annual Gas Production	1.41 x 10 <sup>9</sup> std m <sup>3</sup>	2.12 x 10 <sup>9</sup> std m <sup>3</sup>	2.82 x 10 <sup>9</sup> std m <sup>3</sup>
	(5.25 x 10 <sup>10</sup> SCF)	(7.88 x 10 <sup>10</sup> SCF)	(1.05 x 10 <sup>11</sup> SCF)
Production Cost	6.57¢/std m <sup>3</sup>	5.15¢/std m <sup>3</sup>	4.46¢/std m <sup>3</sup>
	(\$1.77/MSCF)	(\$1.39/MSCF)	(\$1.20/MSCF)
			3.17 x 10 <sup>9</sup> std m <sup>3</sup>
			(1.18 x 10 <sup>11</sup> SCF)
			4.23¢/std m <sup>3</sup>
			(\$1.14/MSCF)

The cost of hydrogen production, in a dual product plant, cannot be explicitly determined. The cost allocations between the hydrogen and methane product streams can be made in a number of equally valid ways. Therefore, it is appropriate to view the production costs in a parametric fashion, i.e., the cost of hydrogen as a function of the value of the co-product methane. Figure 4.3.7 presents the hydrogen production cost in that way.

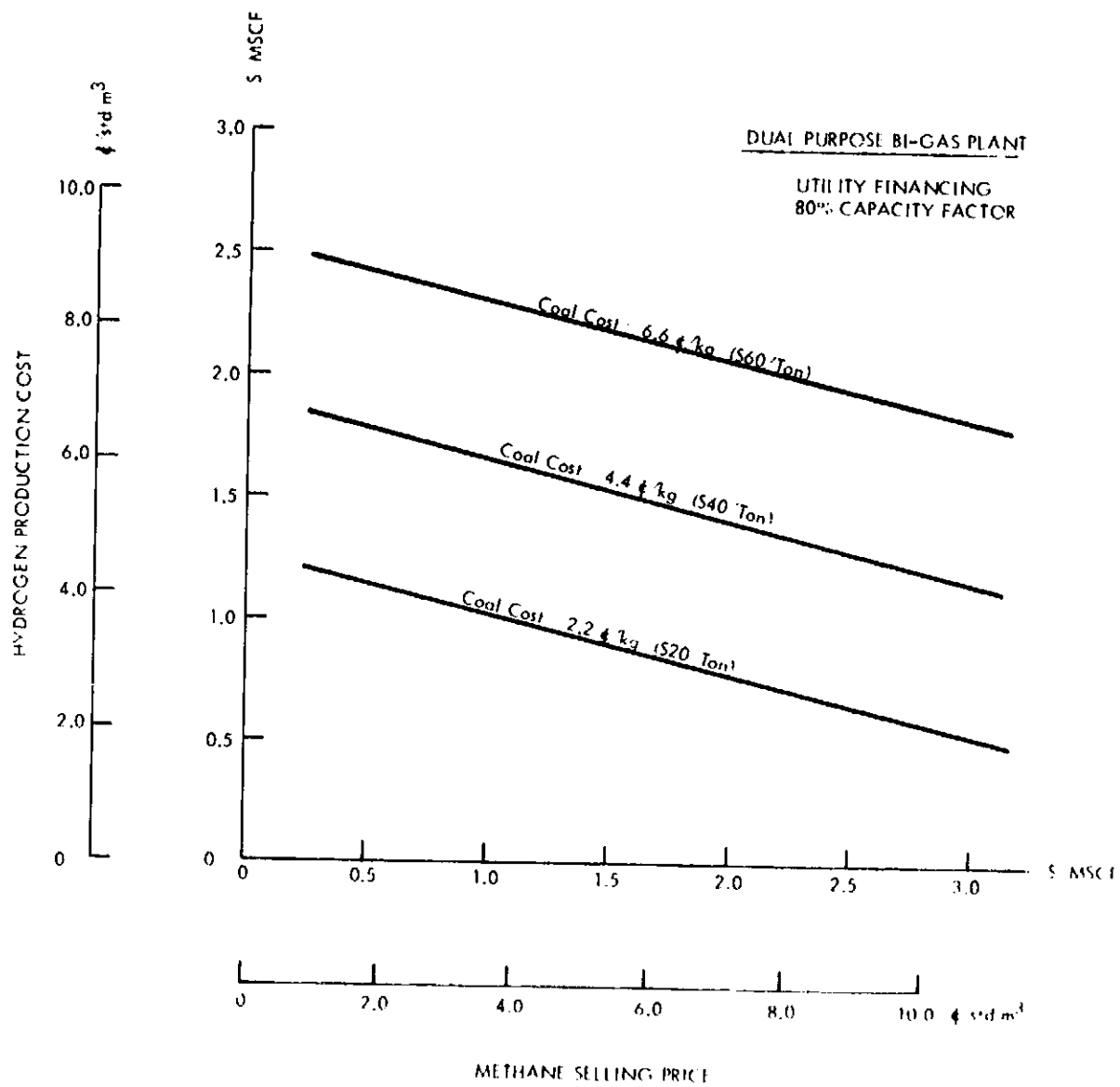


Figure 4.3.7 Hydrogen Production Cost Versus Methane Selling Price

TABLE 4.3.12

DUAL PURPOSE ALTERNATIVE BI-GAS GASIFICATION  
HYDROGEN AND METHANE PRODUCTION COST ESTIMATE  
(80% Capacity Factor)

	Ownership	
	Utility	Industrial
<u>Annual Costs</u>		
Non-Depreciating Capital	\$ 100,000	\$ 100,000
Depreciating Capital	53,557,000	89,012,000
Operation and Maintenance	10,948,000	10,948,000
"Fuel"	67,846,000	67,846,000
<u>Total Annual Cost</u>	<u>\$132,451,000</u>	<u>\$167,906,000</u>
<u>Annual Gas Production</u>		
Hydrogen	$2.82 \times 10^9 \text{ std m}^3$ ( $1.05 \times 10^{11}$ SCF)	$2.82 \times 10^9 \text{ std m}^3$ ( $1.05 \times 10^{11}$ SCF)
Methane	$6.66 \times 10^8 \text{ std m}^3$ ( $2.48 \times 10^{10}$ SCF)	$6.66 \times 10^8 \text{ std m}^3$ ( $2.48 \times 10^{10}$ SCF)
<u>Production Cost</u>	<u>\$2.14/GJ</u> ( <u>\$2.26/10<sup>6</sup> Btu</u> )	<u>\$2.72/GJ</u> ( <u>\$2.87/10<sup>6</sup> Btu</u> )



## 4.4 KOPPERS-TOTZEK COAL GASIFICATION

### 4.4.1 General

Koppers-Totzek gasification is a commercially available process which is adaptable to the production of:

- Synthesis gas for hydrogen, ammonia, methanol, methane, or gasoline.
- Low-Btu fuel gas for various applications, including gas turbines and combined cycle power plants.
- Synthetic natural gas.
- Gases rich in hydrogen and carbon monoxide for direct reduction of ores or for supplemental fuel for blast furnaces.

The Koppers-Totzek concept, i.e., the entrained concurrent flow principle based on the partial combustion of pulverized coal in oxygen and steam, was developed by Dr. F. Totzek of Koppers-Essen. In 1948, Koppers-Essen and Koppers-Pittsburgh, in a joint effort, used this concept in the design of a one ton per hour pilot plant gasifier. The pilot plant was built for the U. S. Bureau of Mines at Louisiana, Missouri, and the first successful run of the gasifier was made on May 4, 1949. The pilot plant was operated over a period of two years to yield liquid hydrocarbon from the Koppers-Totzek synthesis gas.

The first commercial Koppers-Totzek gasifier was installed in Finland in 1952 and was followed by plants in Japan, Spain, Belgium, Portugal, Greece, United Arab Republic, Thailand, Turkey, East Germany, Zambia, South Africa and India. Table 4.4.1 shows a recent list of gasification plants using the Koppers-Totzek process.

### 4.4.2 The Koppers-Totzek Process (References 35, 36 37)

The Koppers-Totzek process, shown in Figure 4.4.1, is based on the partial oxidation of carbonaceous material in the presence of oxygen and steam. For a coal feedstock, a suspension of dry, pulverized coal is carried in a stream of oxygen and steam to a gasifier where it is partially oxidized. The reaction occurs almost completely and instantaneously; carbon conversion is a function only of the reactivity of the coal and approaches 100 percent for lignites. Coal particles do not agglomerate during the plastic stage because the very high temperature zone rapidly decomposes any hydrocarbons formed during gasification. As a result, any coal can be gasified regardless of caking property, ash content, or ash fusion temperature.

TABLE 4.4.1

## GASIFICATION PLANTS USING THE KOPPERS-TOTZEK PROCESS

	Fuel	Number Of Gasifier Units	Capacity: CO - H <sub>2</sub> In 24 Hours	Use Of Synthesis Gas	Year Of Order
Charbonnages de France, Paris Maxingarbe Works (P.D.C.) France	Coal Dust, Coke-Oven-Gas, Tall Gas	1	75,000 - 150,000 Nm <sup>3</sup> 2,700,000 - 5,580,000 SCF	Methanol- and Ammonia Synthesis	1949
Tampere Oy, Oulu Finland	Coal Dust, Oil, Peat	3	140,000 Nm <sup>3</sup> 5,210,000 SCF	Ammonia Synthesis	1950
Nihon Suiso Kagaku Kaisha, Ltd., Tokyo Japan	Coal Dust	3	210,000 Nm <sup>3</sup> 7,820,000 SCF	Ammonia Synthesis	1954
Empresa Nacional "Carbo Sotelo" de Combustibles Líquidos y Lubricantes, S.A., Madrid, Ningun Works in Puentes de García Rodríguez, Coruña Spain	Lignite Dust	3	242,000 Nm <sup>3</sup> 9,000,000 SCF	Ammonia Synthesis	1954
Tampere Oy, Oulu Finland	Coal Dust Oil, Peat	2	140,000 Nm <sup>3</sup> 5,210,000 SCF	Ammonia Synthesis	1955
S.A. Union Chimique Belges, Bussies, Zamevoorde Works Belgium	Bunker-C-Oil Plant Converter for Coal Dust Gasification	2	176,000 Nm <sup>3</sup> 6,550,000	Ammonia Synthesis	1955
América Portuguesa S.A., Lda., Lisbon, Estameiz Plant Portugal	Heavy Gasoline Plant Convertible to Lignite and Anthracite Dust Gasification	2	169,000 Nm <sup>3</sup> 6,100,000	Ammonia Synthesis	1956
The Government of the Kingdom of Greece, The Ministry of Coalmining, Athens, Ningunos Fertilizer Plant, Athens, Greece	Lignite Dust, Bunker-C-Oil	4	679,000 Nm <sup>3</sup> 23,450,000 SCF	Ammonia Synthesis	1959
Empresa Nacional "Carbo Sotelo" de Combustibles Líquidos y Lubricantes, S.A., Madrid, Ningun Works in Puentes de García Rodríguez, Coruña, Spain	Lignite Dust Peat	1	175,000 Nm <sup>3</sup> 6,500,000 SCF	Ammonia Synthesis	1961
The Energy Organization of Greece, the Ministry of Coalmining, Athens, Ningunos Fertilizer Plant, Athens, Greece	Lignite Dust, Coal Dust, Oil, Peat	1	278,000 Nm <sup>3</sup> 28,540,000 SCF	Ammonia Synthesis	1961

TABLE 4.4.1 (Continued)

	Fuel	Number Of Gasifier Units	Capacity: CO - H <sub>2</sub> In 24 Hours	Use Of Synthesis Gas	Year Of Order
Chemical Fertilizer Company, Ltd., Trinidad; Synthetic Fertilizer Plant at Moe Mah, Lebanon; Trinidad	Lignite Dust	1	217,000 Nm <sup>3</sup> 8,070,000 SCF	Ammonia Synthesis	1963
Azot Sarayli T.A.S., Ankara, Turkey	Lignite Dust	4	775,000 Nm <sup>3</sup> 28,850,000	Ammonia Synthesis	1966
Chemiesingen Export-Import G.m.b.H., Berlin for VEB Germania, Chemiesingen and Apparatebau, Halle-Merseburg; VEB Zeitz-Werk	Vacuum Residue and or Fuel Oil	2	360,000 Nm <sup>3</sup> 13,400,000 SCF	Raw Gas to Produce Hydrogen for Hydrogen Generation	1966
Kobe Steel, Ltd., Kobe Japan for Industrial Development Corp., Zambia, at Kafue near Lusaka Zambia, Africa	Coal Dust	1	214,320 Nm <sup>3</sup> 7,980,000 SCF	Ammonia Synthesis	1967
Endogenous Fertilizers Industry, S.A., Athens	Lignite Dust	1	165,000 Nm <sup>3</sup> 6,150,000	Ammonia Synthesis	1969
Endogenous Fertilizers Plant, Proemati, Greece	Coal Dust	3	2,000,000 Nm <sup>3</sup> 74,450,000 SCF	Ammonia Synthesis	1969
The Fertilizer Corporation of India Ltd., New Delhi; Sangamdam Plant, India	Coal Dust	3	2,000,000 Nm <sup>3</sup> 74,450,000 SCF	Ammonia Synthesis	1970
The Fertilizer Corporation of India Ltd., New Delhi; Talyer Plant, India	Lignite Dust	1	242,000 Nm <sup>3</sup> 9,009,000 SCF	Ammonia Synthesis	1972
Endogenous Fertilizers Industry, S.A., Athens	Coal Dust	3	2,000,000 Nm <sup>3</sup> 74,450,000	Ammonia Synthesis	1972
Endogenous Fertilizers Plant, Proemati, Greece	Coal Dust	3	2,150,060 Nm <sup>3</sup> 80,125,000 SCF	Ammonia Synthesis	1972

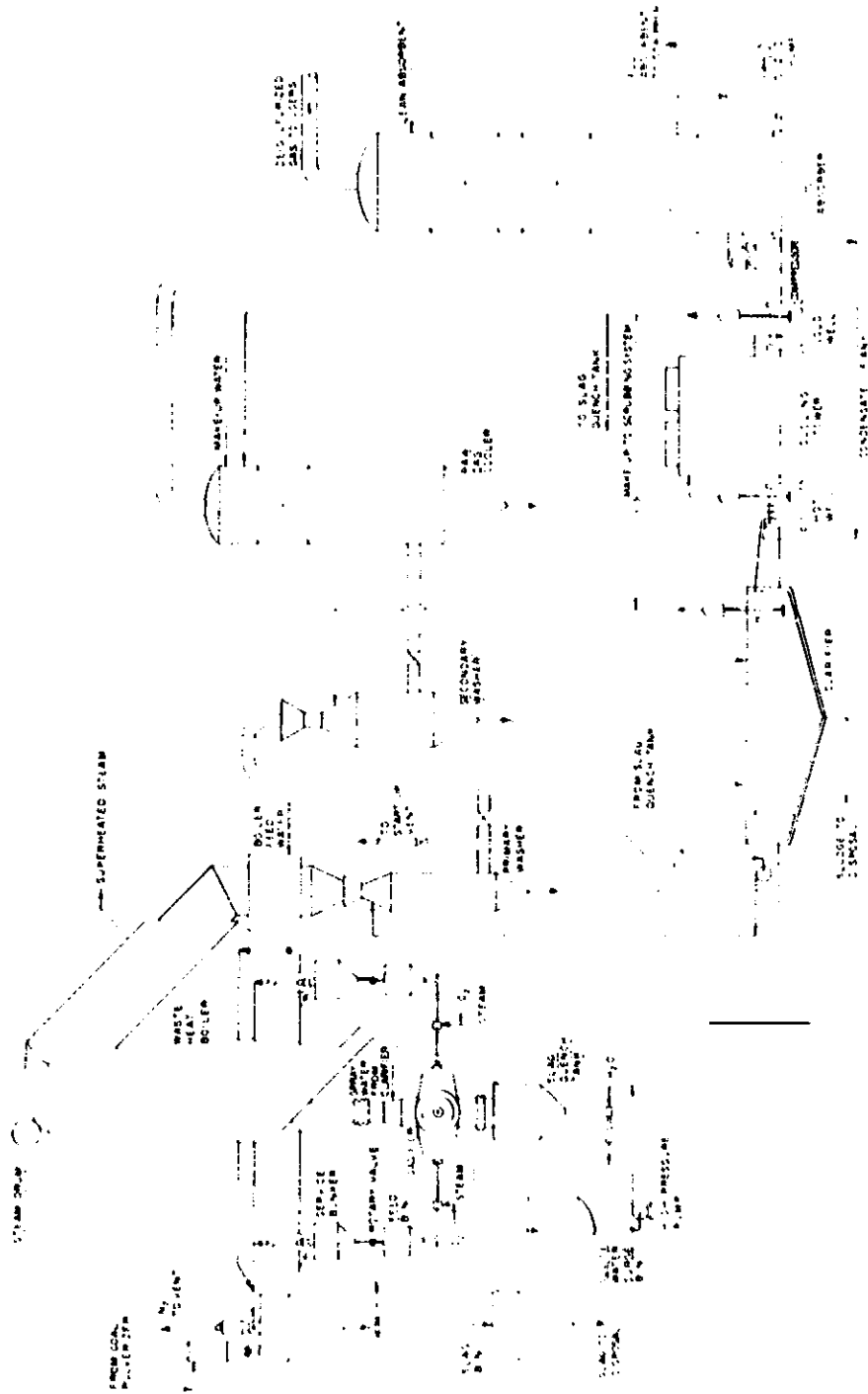


Figure 4.4.1 Koppers-Totzek Gasification Process

Raw coal is dried to a moisture content of between 2 and 8 percent, depending on the rank of the coal, and pulverized to about 70 percent through 200 mesh. This dry coal dust is carried in a nitrogen stream to a service bunker prior to distribution to gasifier feed bins. From the bins, screw feeders discharge the coal dust into a stream of oxygen and low-pressure steam which carries the coal to the gasifier. Moderate temperature and high burner velocity prevent the coal from being oxidized prematurely.

The heart of the Koppers-Totzek gasification process is the gasifier. Koppers offers both a two-headed gasifier capable of handling 15000 kg/hr (400 tpd) of coal and a four-headed gasifier capable of handling 32000 kg/hr (850 tpd). In the two-headed gasifier, Figure 4.4.2, burner heads are 180 degrees apart; in the four-headed gasifier, they are 90 degrees apart. The gasifier, shaped like spheroidal cones centrally welded together, has a double-walled shell constructed of boiler quality plate. The annulus between inner and outer shell is water-cooled and connected to a steam separation drum. The low-pressure steam generated in the double-walled shell is used as the process steam which enters the gasifier through the mixing heads.

At the apex of each gasifier cone is mounted a set of burners in line with an opposing set. Advantages of opposing burners are that projected particles which pass through their own flame region unburned are gasified in the opposing flame, and as the flame is directed into a gaseous medium, refractory problems with instantaneous high temperatures are minimized.

Entering the gasifier, carbon in the entrained oxygen-steam stream is exothermically oxidized, producing a high temperature flame zone in the region of about 2200K (3500°F). Endothermic reactions between the carbon and steam substantially reduce the flame temperature to around 1755K (2700°F), while continuing in the process to oxidize carbon and produce additional hydrogen.

As the gas leaves the gasifier, it is water quenched to solidify any entrained slag; sensible heat is recovered via a waste heat boiler which produces high-pressure steam. This steam may be used for turbine drives for compressors or pumps.

At entry to the waste heat boiler, theoretical equilibrium calculations show essentially all hydrocarbons, including phenols and tars, and ammonia, etc., to be dissociated and oxidized. In practice, the gas is essentially carbon monoxide, hydrogen and carbon dioxide with a relatively small percentage of nitrogen, hydrogen sulfide, and carbonyl sulfide and only trace quantities of other compounds.

The gas is then passed through a scrubbing system to reduce entrained solids to  $4.6 \times 10^{-6} \text{ kg/m}^3$  (0.002 grains/scf) and to lower the temperature to about 308K (95°F).

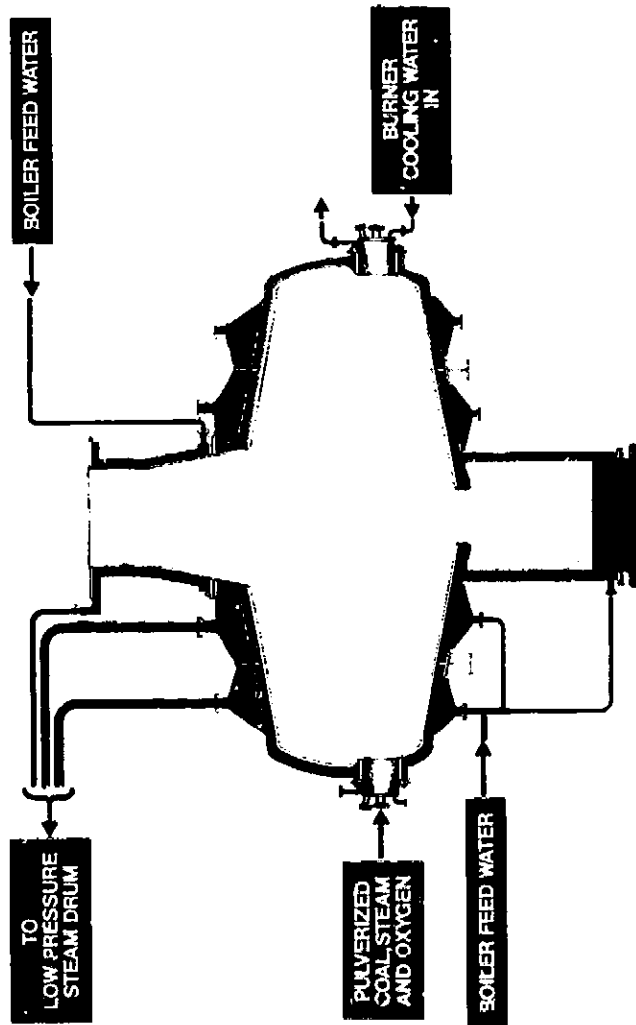


Figure 4.4.2 Two Heded Koppers-Totzek Gasifier

Particulate-laden recirculated water from the gas cleaning and cooling system is piped to a clarifier. The sludge from the clarifier is pumped either to a filter or the plant disposal area. The clarified water is pumped to a cooling tower and is recirculated through the gas cleaning system. A small quantity of make-up water is required to compensate for evaporation, windage, and blowdown losses at the cooling tower, as well as moisture losses in the clarifier sludge and slag.

The synthesis gas, subsequent to cleaning and cooling, is processed in the manner consistent with the desired end product. For the generation of a hydrogen product, the processing steps include sulfur and acid gas removal, carbon monoxide shift, carbon dioxide removal, and polishing methanation.

There are several features of the Koppers-Totzek process that makes it particularly attractive for hydrogen generation from coal. First and foremost is that it is a commercially successful system. As such, the technology of the process, including materials requirements, operating procedures, and performance characteristics are both well known and predictable. In addition, the downstream processing steps use known technologies, commercially available catalysts, and predictable performance and economics.

The Koppers-Totzek process also has considerable flexibility in the choice of fuel to be gasified. The Koppers-Totzek process can continuously gasify a wide range of feedstocks including all types of coal, char, petroleum, coke, tars, heavy residuals, light and heavy oils, and even slurries of carbonaceous materials in hydrocarbon liquids. For coal feedstock, coal size is not a limiting factor and coking coals can be handled without pretreatment. The process is totally independent of the fuel's volatile content, its caking and swelling properties, its ash content, and its ash-fusion temperature.

Two other advantages of the Koppers-Totzek process are pollution-free operation and safety.

Because of the high reaction temperature and the high exit-gas temperature, the only products are gas and slag. The gas is free of tars and condensable hydrocarbons and complex organic sulfur compounds; contaminants such as cyanides, phenols, and ammonia are reduced to trace quantities. About 50 percent of the ash drains from the gasifiers as molten slag into a water quench; the remainder is removed in the gas cleaning and cooling system.

The Koppers-Totzek process has over 20 years of safe operation. Failure of any component automatically closes down all other systems and purges the gasification system with nitrogen. All bins and tanks are blanketed with nitrogen under pressure to eliminate any explosion hazard.

The disadvantages of the Koppers-Totzek process relate primarily to the capacity and operating pressure of the gasifiers. The former results in a multiplicity of units for large plants, affecting the capital cost of the facility. The latter relates to the additional capital and operating costs that are involved in compression work if the process gas is to be delivered at elevated pressures.

There are privately funded programs underway to minimize the detrimental effects of these disadvantages. Figure 4.4.3 shows the progression in capacity of the two headed gasifiers, from the early designs of 54 std m<sup>3</sup>/min (2000 SCFM) to the present 348 std m<sup>3</sup>/min (13000 SCFM). Four-headed gasifiers have presently projected capacities in the region of 32,000 kg hr (850 tpd) of coal or around 900 std m<sup>3</sup>/min (33,000 SCFM) of gas.

A small pressurized entrained gasifier, designed for up to 3040 kPa (30 atm) operation, has been tested at the Dusseldorf Research Center of Koppers-Essen. These tests have been sufficiently successful to indicate that commercial operation at pressure is feasible. The advantages claimed for operation at pressures over the present atmospheric gasifier are for those processes involving hydrogen, ammonia, methanol, methane generation, or combined cycle operations. The advantages include a substantial capital and operating savings in the cost of gas compression, a more compact design, improved gas cleaning, and improved carbon conversion. The disadvantages include a loss of simplicity of gasifier design and operation, and the need to design for higher erosion from more concentrated dust and particulate loadings.

#### 4.4.3 Hydrogen Production Plant

##### 4.4.3.1 General

The design of the hydrogen production plant was based on the use of a process configuration that employs the appropriate processing steps to achieve a high purity hydrogen product stream. The principal operating characteristics of the plant are shown in Table 4.4.2 and the overall summary process flowsheet is portrayed in Figure 4.4.4. The sections below discuss the individual process steps, as well as some of the plant support facilities, resource requirements, and performance considerations.

##### 4.4.3.2 Coal Preparation

Coal preparation considers all those steps from receipt of coal on-site to distribution to the gasifiers and steam boilers. Included are items such as unloading, coal storage, drying and pulverizing.

It is assumed, for purpose of the evaluation, that coal is delivered to the site by rail. The coal, as delivered, has already undergone preparation at the mine to remove rock and overburden and has been screened to remove oversized pieces.



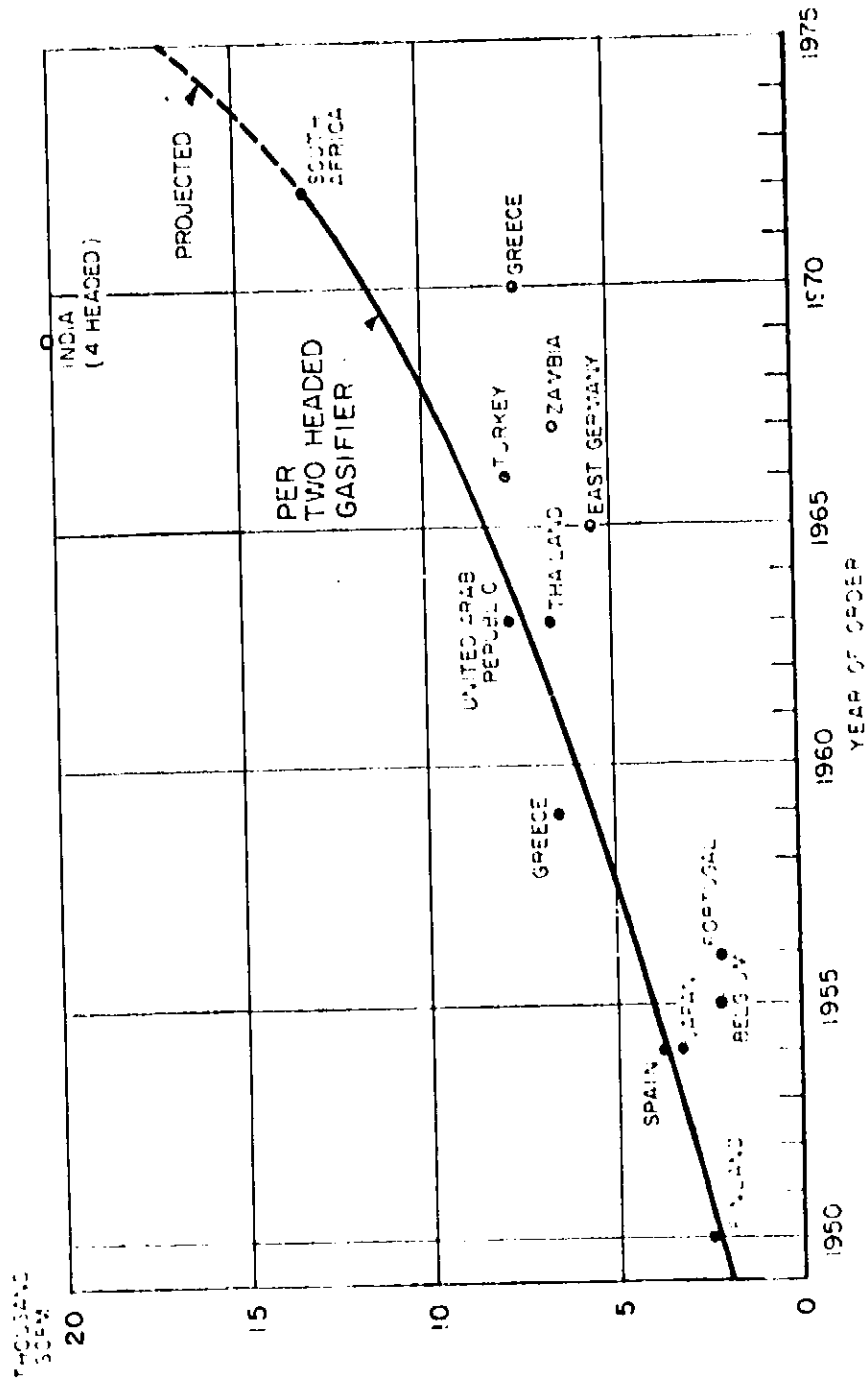
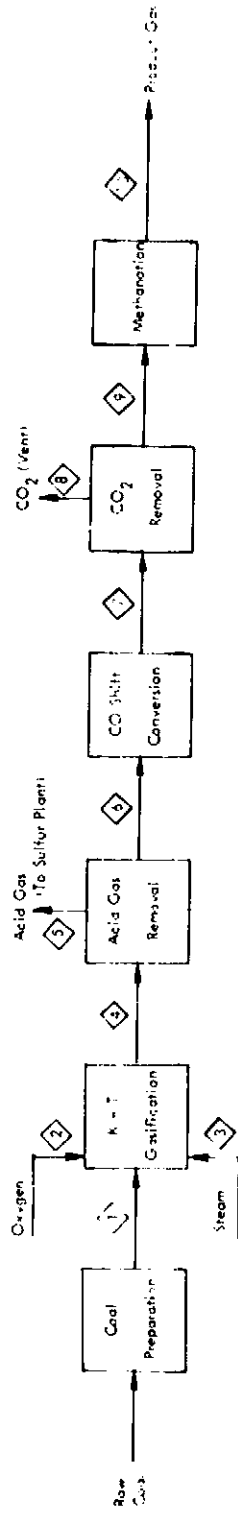


Figure 4.4.3 Koppers Coal Gasification Process Dry Gas Production Capacity  
(Chronological Order)



OVERALL PROCESS BALANCE

STREAM NO.	1	2	3	4	5	6	7	8	9	10
STREAM NAME	COAL FEED	OXYGEN FEED	STEAM FEED	ACID GAS REMOVAL FEED	ACID GAS	CO SHIFT FEED	CO2 REMOVAL FEED	CO2 VENTED	VENTILATION FEED	PRODUCT GAS
	LB HR	K MOLE HR	K MOLE HR	K MOLE HR	K MOLE HR	LB MOLE HR	K MOLE HR	K MOLE HR	K MOLE HR	K MOLE HR
1	24,380			6,972		6,564	18,713			
2	24,380	24,817		12,283	3.2	12,274	526			
3			1,377	1,377	3.223	Trace	11,748	11,722		
4				247		240	240			
5										
6				300	826					
7				27,178	4,143	35,487	31,273	68,863	111,702	25,729
8				1,225	2,172	2,024	29,534	61,463		
9				27,672	4,911	29,804	64,831	134,376	11,702	25,729
10				20,011	41,144	18,671	18,244	44,111	1,145	1,145
TOTAL	24,380	24,817	1,377	44,632	8,226	18,819	51,113	111,702	11,702	25,729
NET	24,380	24,817	1,377	1,377	1,377	1,377	2,456,739	3,126,111	3,126,111	3,126,111
PERCENTAGE	100	100	100	100	100	100	100	100	100	100
PERCENTAGE	100	100	100	100	100	100	100	100	100	100

Figure 4.4.4 Hydrogen Production Using Koppers-Totzek Coal Gasification

TABLE 4.4.2  
KOPPERS-TOTZEK GASIFICATION PLANT  
PRINCIPAL OPERATING CHARACTERISTICS

Type of Gasifier	4 Headed
Number of Operating Gasifiers	10
Capacity of Gasifier	857 std m <sup>3</sup> /min (32,000 SCFM)
Gasifie. Operating Pressure	Atmospheric
Plant Output	9.56 x 10 <sup>6</sup> std m <sup>3</sup> /day (357 x 10 <sup>6</sup> SCFD)
Hydrogen Purity	95.4 %
Coal Feed to Gasifiers (Dry)	261,000 kg/hr (287 Tons/Hr)
Product Gas Pressure	6895 kPa (1000 psi)
Overall Process Efficiency	49 %

TABLE 4.4.3  
COAL CHARACTERISTICS (AS RECEIVED)

Carbon	62.98 %
Hydrogen	4.23 %
Nitrogen	1.22 %
Sulfur	4.23 %
Oxygen	7.90 %
Ash	13.63 %
Moisture	6.00 %
Heating Value	26.36 MJ/kg (11,340 Btu/lb)

The coal used in the process has the characteristics as shown in Table 4.4.3. The coal preparation facilities are sized, with margin, to handle the coal consumption rate of the gasifiers and the boilers for production of steam, in excess of that produced in the gasifiers, for the oxygen plant, gas compressors, shift converters, and other uses. The normal coal consumption, and delivery rate, is  $9.6 \times 10^6$  kg/day (10585 tpd), made up of  $6.6 \times 10^6$  kg/day (7324 tpd) for gasification and  $3 \times 10^6$  kg/day (3261 tpd) for other uses. A sixty day coal storage pile provides the flexibility for continued operation in spite of possible delivery delays.

Coal is prepared by drying and pulverization to about 70 percent through 200 mesh in a wind swept closed system using ball, rod, or roller mills. The degree of drying is generally a function of the material to be pulverized, varying from 2 to 8 percent.

#### 4.4.3.3 Gasification

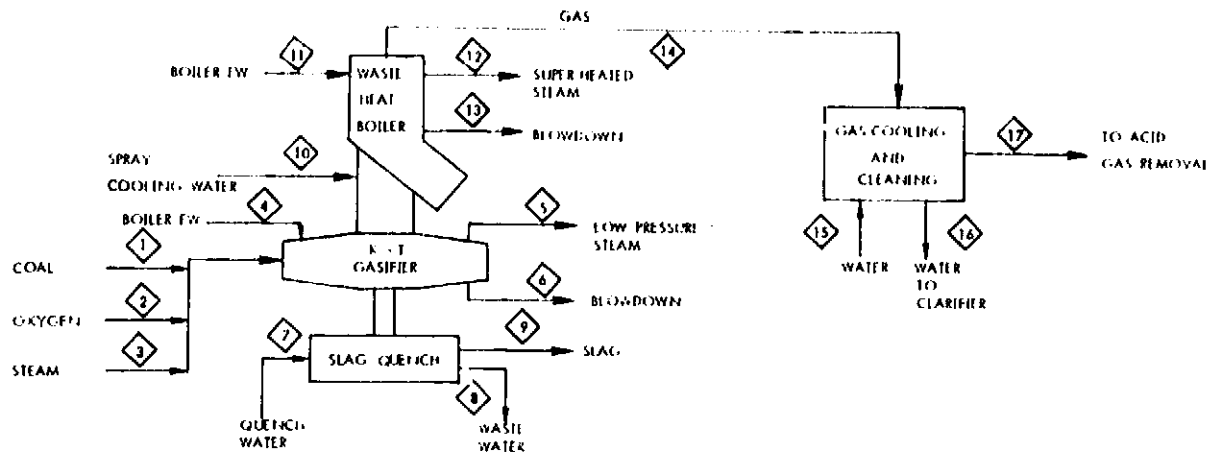
The flowsheet for the Koppers-Totzek gasification step is shown in Figure 4.4.5. Two gasifiers, operating in parallel, are required to meet the full product output. The gasification step includes heat recovery from the gasifiers in both the shell of the gasifier proper and the waste heat boiler. The steam thus produced is used, in conjunction with steam produced in coal fired boilers, to meet the plant's overall steam needs. A gas cleaning and cooling section is included in the flow diagram in order to remove fine ash and dust carried over in the gas stream and to reduce the temperature of the synthesis gas to 311K (100°F). The gross thermal efficiency of the gasification step, defined as the calorific value of the synthesis gas divided by the heat content of the coal fed to the gasifier, is approximately 71 percent.

#### 4.4.3.4 Acid Gas Removal

The acid gas removal step shown in Figure 4.4.6 is for the purpose of removing CO<sub>2</sub> and sulfurous compounds from the product stream. Prior to processing, the gas is compressed to 1410 kPa (205 psia) from the essentially atmospheric discharge of the gasifier. Final compression to the plant discharge pressure is done further downstream. Elemental sulfur, at the rate of approximately 11,700 kg/hr (310 tpd) is extracted from the acid gas in the sulfur plant. If this sulfur can be sold, a credit against the cost of hydrogen production can be achieved. Assuming a sales price of 2.2¢/kg (\$20/ton), this credit would be in the order of 0.06¢ m<sup>3</sup> (1.7¢/MSCF).

#### 4.4.3.5 CO Shift Conversion

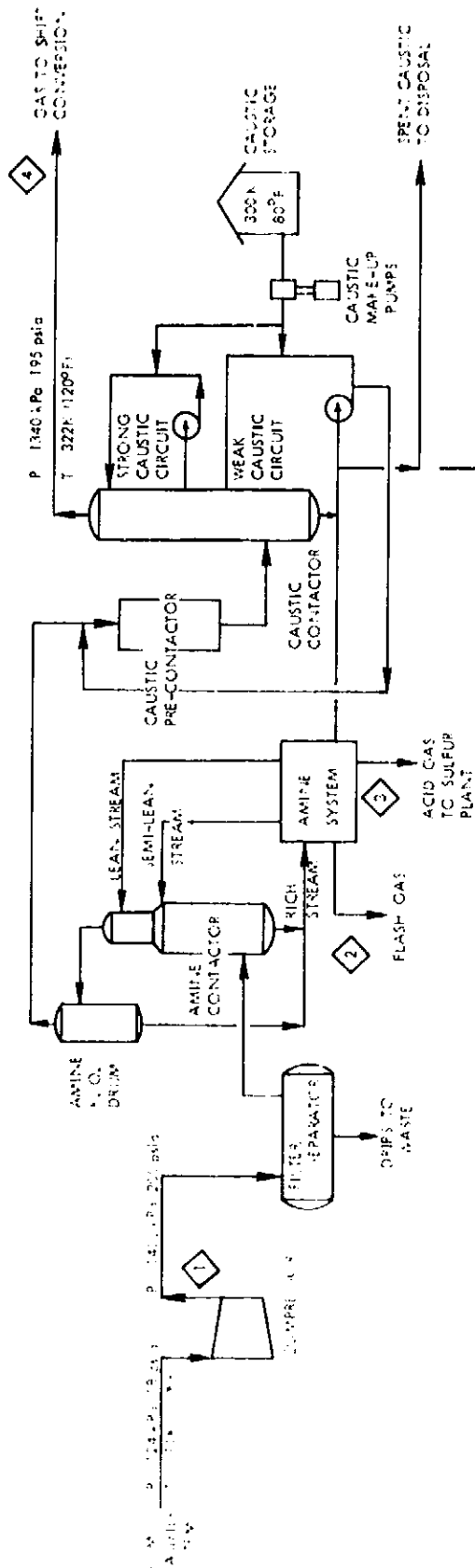
The CO shift conversion, Figure 4.4.7, catalytically converts CO to CO<sub>2</sub>, by the addition of steam, with the resultant production of additional hydrogen gas according to the reaction  $\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$ . Secondary compression is applied in this step to



STREAM NO.	1	2	3	4	5	6	7	8	9
STREAM NAME	COAL FEED	OXYGEN	STEAM	BOILER FW	L. P. STEAM	BLOWDOWN	QUENCH WATER	WASTE WATER	SLAG
	MOL WT	KG HR	LB HR	KG Mole Hr	LB Mole Hr	KG Mole Hr	LB Mole Hr	KG Mole Hr	LB Mole Hr
C	12.01	174,260	384,391						
H <sub>2</sub>	2.016	11,711	25,817						
CO	28.01								
CO <sub>2</sub>	44.01								
CH <sub>4</sub>	16.042								
H <sub>2</sub>	2.016	11,711	25,817	127	279				
S	32.06	11,711	25,817						
O <sub>2</sub>	32.00	21,972	48,219	6,201	13,670				
H <sub>2</sub> S	34.076	400							
ASH	12.01	21,972	48,219						
Total (Dry)		298,343	648,347	6,328	13,942				
H <sub>2</sub> O	18.015	11,711	25,817	4,728	10,424				
Total Wet		310,054	674,164	11,056	24,366				
Elemental Fe				179 (223)	400 (277)				
Elemental Fe (lb)				380	880				
Elemental Fe (kg)				172	400				
Water (kg)				11,711	25,817				
Water (lb)				25,817	57,219				
Water (M <sup>3</sup> )				117.11	258.17				
Water (GPM)				1,171.1	2,581.7				
Water (GPD)				28,106	61,961				
Water (MGD)				0.281	0.620				

STREAM NO.	10	11	12	13	14	15	16	17
STREAM NAME	SPRAY WATER	BOILER FW	SUPER HEATED STEAM	BOILER BLOWDOWN	WASTE HEAT BOILER BLOWDOWN	WATER TO CLARIFIER	WASTE WATER TO CLARIFIER	TO ACID GAS REMOVAL
	MOL WT	KG HR	LB HR	KG Mole Hr	LB Mole Hr	KG Mole Hr	LB Mole Hr	KG Mole Hr
C	12.01							
H <sub>2</sub>	2.016							
CO	28.01							
CO <sub>2</sub>	44.01							
CH <sub>4</sub>	16.042							
H <sub>2</sub>	2.016							
S	32.06							
O <sub>2</sub>	32.00							
H <sub>2</sub> S	34.076							
ASH	12.01							
Total (Dry)								
H <sub>2</sub> O	18.015							
Total Wet								
Elemental Fe								
Elemental Fe (lb)								
Elemental Fe (kg)								
Water (kg)								
Water (lb)								
Water (M <sup>3</sup> )								
Water (GPM)								
Water (GPD)								
Water (MGD)								

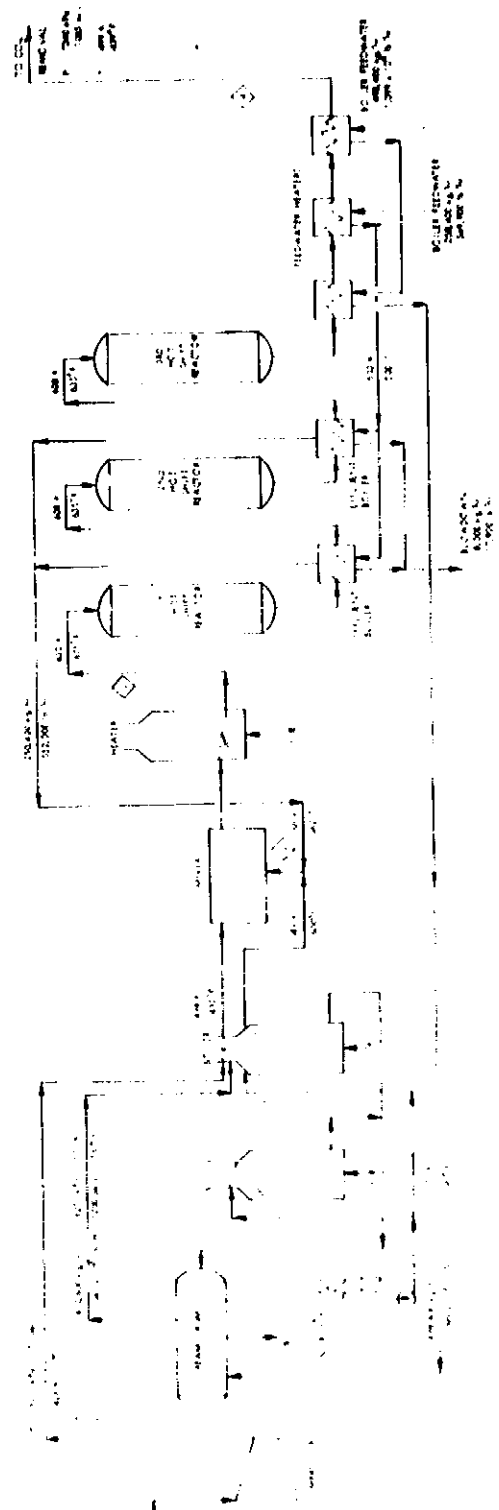
Figure 4.4.5 Hydrogen Production Using Koppers-Totzek Gasification - Gasification Step



ACID GAS REMOVAL BALANCE

STREAM NO.	1		2		3		4		
	FEED GAS		FLASH GAS		ACID GAS		TO SHIFT CONVERSION		
STREAM NAME	K Mole/Hr	Lb Mole/Hr	K Mole/Hr	Lb Mole/Hr	K Mole/Hr	Lb Mole/Hr	K Mole/Hr	Lb Mole/Hr	
H <sub>2</sub>	2,216	6,972	15,371	5	11	3	7	6,964	15,353
CO	28,31	12,264	27,583	6	13	3	7	12,275	27,060
CO <sub>2</sub>	42,33	1,507	3,323	-	-	1,507	3,323	Trace	Trace
CH <sub>4</sub>	16,342	-	-	-	-	-	-	-	-
H <sub>2</sub> O	26,12	245	545	-	-	-	-	249	549
N <sub>2</sub>	34,35	366	806	-	-	366	806	Trace	Trace
Total-Dry	-	21,578	47,129	11	24	1,672	4,143	19,488	42,942
H <sub>2</sub> O	15,12	1,273	2,572	23	50	16	36	1,317	2,904
Total-Wet	-	22,635	49,701	34	74	1,688	4,179	20,805	45,846
Molecular Wt.	-	73,01	11,3	24,6	1,955	4,311	20,805	45,856	18,67
Mass Flow Rate	-	1,662,500	41,13	235	80,200	388,400	1,76,900	856,400	656,400
Flow Rate	-	1,226,400	295	295	176,900	176,900	176,900	176,900	176,900
Conversion %	-	-	-	-	-	-	-	-	-
CFD	-	14.7 * 10 <sup>6</sup>	6,300	1.05 * 10 <sup>6</sup>	1.05 * 10 <sup>6</sup>	39.3 * 10 <sup>6</sup>	11.2 * 10 <sup>6</sup>	417.7 * 10 <sup>6</sup>	417.7 * 10 <sup>6</sup>

Figure 4.4.6 Hydrogen Production Using Koppers-Totzek Coal Gasification Acid Gas Removal Step



ITEM	UNIT	QTY	DESCRIPTION
1	KG	1000	WATER
2	KG	200	20% NaOH
3	KG	200	20% NaOH
4	KG	200	20% NaOH
5	KG	100	CO2
6	KG	100	CO2
7	KG	100	CO2
8	KG	100	CO2
9	KG	100	CO2
10	KG	100	CO2
11	KG	100	CO2
12	KG	100	CO2
13	KG	100	CO2
14	KG	100	CO2
15	KG	100	CO2
16	KG	100	CO2
17	KG	100	CO2
18	KG	100	CO2
19	KG	100	CO2
20	KG	100	CO2
21	KG	100	CO2
22	KG	100	CO2
23	KG	100	CO2
24	KG	100	CO2
25	KG	100	CO2
26	KG	100	CO2
27	KG	100	CO2
28	KG	100	CO2
29	KG	100	CO2
30	KG	100	CO2
31	KG	100	CO2
32	KG	100	CO2
33	KG	100	CO2
34	KG	100	CO2
35	KG	100	CO2
36	KG	100	CO2
37	KG	100	CO2
38	KG	100	CO2
39	KG	100	CO2
40	KG	100	CO2
41	KG	100	CO2
42	KG	100	CO2
43	KG	100	CO2
44	KG	100	CO2
45	KG	100	CO2
46	KG	100	CO2
47	KG	100	CO2
48	KG	100	CO2
49	KG	100	CO2
50	KG	100	CO2

Figure 4.4.7 Hydrogen Production Using K-T Coal Gasification - CO Shift Step

raise the product gas pressure to levels sufficiently high to assure a final product gas pressure of 68905 kPa (1000 psia).

Steam for the shift conversion is produced by a combination of coal fired boilers and recovered heat from the exothermic shift reaction.

#### 4.4.3.6 CO<sub>2</sub> Removal

The CO<sub>2</sub> removal step, Figure 4.4.8, results in a process gas that contains 95.8% H<sub>2</sub>, 2.7% CO, 0.2% CO<sub>2</sub> and 1.3% N<sub>2</sub>. Depending upon the ultimate use of the gas, the output from this step might be considered as the final product from the process. However, since the hydrogen is, by definition, not destined for a specific application but rather distributed by pipeline to off-site consumers, it is desirable to incorporate an additional step to remove the CO from the gas to assure its environmental acceptability in case of leakage.

#### 4.4.3.7 Polishing Methanation

This step, shown in Figure 4.4.9, catalytically converts the CO and CO<sub>2</sub> to methane (CH<sub>4</sub>) and water in accordance with the reactions:



The product gas now consists of 95.4% H<sub>2</sub>, 3.2% CH<sub>4</sub>, 1.4% N<sub>2</sub>, and trace amounts of water, CO, and CO<sub>2</sub>. The higher heating value of the process gas is 12.77 MJ/m<sup>3</sup> (343 Btu/SCF).

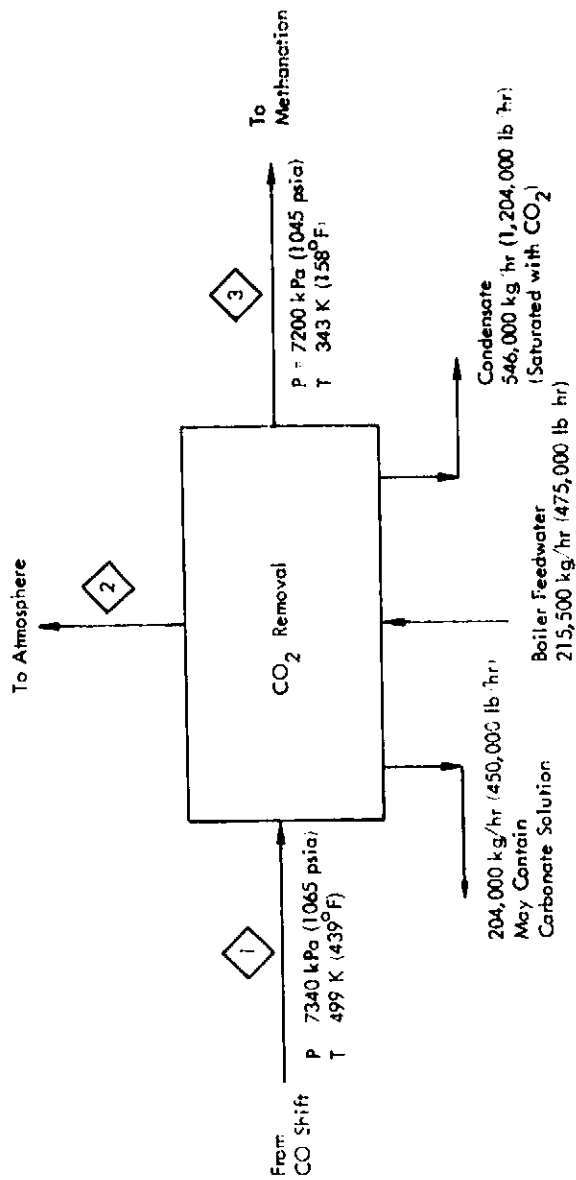
#### 4.4.3.8 Plant Service Systems

Associated with, and supporting the operation of the process plant are a number of service systems. These include such items as the oxygen plant, cooling water, water make-up, waste disposal, steam generation, electrical distribution, and the plant administrative, maintenance, and support facilities.

##### 4.4.3.8.1 Oxygen Plant

The oxygen plant provides a gas stream to the Koppers-Totzek gasifiers containing 98 percent oxygen and 2 percent nitrogen. The nominal flow rate, at full plant capacity, is 202,000 kg/hr (445,100 lb/hr).



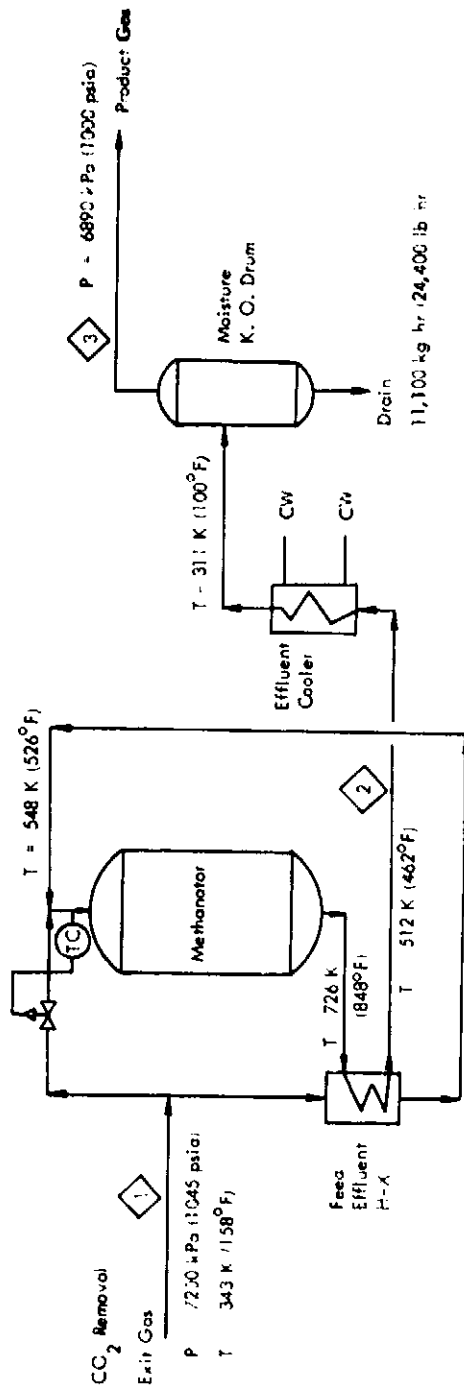


CO<sub>2</sub> REMOVAL BALANCE

Stream No.	Stream Name	CO Shift Exit		CO <sub>2</sub> Removed		Gas To Methanation	
		K Mole/Hour	Lb Mole/Hour	K Mole/Hour	Lb Mole/Hour	K Mole/Hour	Lb Mole/Hour
H <sub>2</sub>	2,016	18,713	41,254	-	-	18,713	41,254
CO	28,01	526	1,159	-	-	526	1,159
CO <sub>2</sub>	44,01	11,749	25,901	11,702	25,797	47	104
CH <sub>4</sub>	16,042	-	-	-	-	-	-
N <sub>2</sub>	28,02	249	549	-	-	249	549
Total (Dry)	-	31,237	68,863	11,702	25,797	19,535	43,066
H <sub>2</sub> O	18,016	29,694	65,463	-	-	-	-
Total (Wet)	-	60,931	134,326	11,702	25,797	19,535	43,066
Molecular Weight:	-	18,24	-	44,01	-	3,148	-
Mass Flow Rate	-	1,111,400	-	515,000	-	61,500	-
Pounds/hr	-	2,450,300	-	1,135,300	-	135,600	-
Volume Flow Rate	-	32.8 x 10 <sup>6</sup>	-	6.29 x 10 <sup>6</sup>	-	10.51 x 10 <sup>6</sup>	-
SCFD	-	1,223 x 10 <sup>6</sup>	-	235 x 10 <sup>6</sup>	-	392.2 x 10 <sup>6</sup>	-

Figure 4.4.8 Hydrogen Production Using Koppers-Totzek Coal Gasification - CO<sub>2</sub> Removal Step

REPRODUCIBILITY OF THE  
ORIGINAL DATA IS GUARANTEED



METHANATION PROCESS BALANCE

Stream No.	1		2		3	
	CC <sub>2</sub> Removal	Methanator Exit	Methanator Exit	Product Gas	Product Gas	Product Gas
Mole Weight	K Mole/Hour	Lb Mole/Hour	K Mole/Hour	Lb Mole/Hour	K Mole/Hour	Lb Mole/Hour
H <sub>2</sub>	2,016	18,713	41,254	16,947	37,361	16,947
CO	28.01	526	1,159	50 ppm	50 ppm	50 ppm
CO <sub>2</sub>	44.01	47	104	50 ppm	50 ppm	50 ppm
CH <sub>4</sub>	16.42	-	-	573	1,263	573
N <sub>2</sub>	28.02	249	549	249	549	249
Total (Dry)	-	19,535	43,066	17,769	39,172	17,769
H <sub>2</sub> O	18.016	-	-	620	1,367	6
Total (wet)	-	19,535	43,066	18,389	40,540	17,775
Molecular Weight	-	3.148	-	3.34	-	2.838
Mass Flow Rate	-	-	-	-	-	-
K G Hr	-	61,507	-	61,507	-	50,442
Pounds Hr	-	135,601	-	135,601	-	111,200
Volume Flow Rate	-	10,31 x 10 <sup>6</sup>	-	9.3 x 10 <sup>6</sup>	-	9.56 x 10 <sup>6</sup>
SCFD	-	152.25 x 10 <sup>6</sup>	-	165.20 x 10 <sup>6</sup>	-	156.90 x 10 <sup>6</sup>

Figure 4.4.9 Hydrogen Production Using Koppers-Totzek Coal Gasification - Methanation Step

#### 4.4.3.8.2 Cooling Water

To minimize the potential environmental impact of the plant, cooling towers are used to dissipate the plant waste heat. The use of cooling towers results in higher capital and operating costs than would occur with direct river cooling, but does result in what is believed will be an environmentally acceptable system.

The wet cooling towers employed perform their cooling function by both the sensible heat transfer from the cooling water to the air plus the evaporative cooling of the water. The water make-up system must provide sufficient fresh cooling water to compensate for the evaporative, windage, and blowdown consumption.

#### 4.4.3.8.3 Water Make-Up

The water make-up system takes river water and treats it as appropriate for the various needs of the plant. Two general levels of water treatment are provided, i.e., a water quality suitable for cooling water uses and a quality suitable for boiler feedwater. The nominal rating of the water make-up system is  $2.87 \times 10^6$  kg/hr ( $6.34 \times 10^6$  lb/hr), made up of:

Boiler Feedwater Quality	$1.12 \times 10^6$ kg/hr ( $2.48 \times 10^6$ lb/hr)
Cooling Water Quality	$1.71 \times 10^6$ kg/hr ( $3.78 \times 10^6$ lb/hr)
Potable Water	$0.14 \times 10^6$ kg/hr ( $0.08 \times 10^6$ lb/hr)

#### 4.4.3.8.4 Steam Generation

Steam is required in several sections of the plant. These include the gasifiers themselves, the oxygen plant, the turbine drives for the primary and secondary product gas compressors, the CO shift reaction, and other process uses. Steam is generated for these uses from several sources.

Steam for the CO shift is generated by a combination of coal fired boilers and recovered heat from the exothermic shift reaction. The remainder of the plant steam requirements are met by separate coal fired boilers and the waste heat steam generation associated with the gasification reaction.

The coal fired boilers used for steam generation use the same kind of coal as the gasifiers. To assure a minimum environmental impact potential, a limestone slurry flue gas cleanup system is included in order to control flyash and SO<sub>2</sub> releases to within acceptable limits.

#### 4.4.3.8.5 Waste Disposal

In accordance with the basic assumption of having the plant meet the environmental discharge regulations that either exist or are expected to exist, facilities and provisions have

been incorporated to handle the waste products from the process. Systems have been included to clean up liquid waste streams and solidify, to the greatest extent possible, the dissolved or suspended wastes for ultimate disposal. It is assumed that ultimate waste disposal will take place off-site, and that only temporary storage facilities are needed at the plant site. An allowance has been included in the plant operation and maintenance cost to account for the fee associated with transportation and ultimate storage of all solid wastes.

#### 4.4.3.8.6 Electrical Distribution

All electric power required for the operation of the plant is generated off-site in an electric utility system and fed to the plant through a 138 kV transmission line. The plant electrical system steps down this voltage and distributes power to the various users within the facility. The total installed plant electric capacity is 67,000 kVA, with the normal full load electrical consumption approximately 42,750 kW.

#### 4.4.4 Plant Performance Characteristics

The performance of the plant can be expressed in several different ways. The paragraphs below summarize the performance in terms of resource consumption process outflows, and overall thermal efficiency.

##### 4.4.4.1 Resource Consumption

For purposes of evaluation, the only resources considered are those associated with the operation of the plant, and not with the manufacture or construction of the facility. The resources are categorized into coal, consumptive water use, electricity, limestone (for flue gas clean-up), and chemicals and catalysts. Table 4.4.4 summarizes the annual consumption of these materials. It should be noted that, for purposes of conservatism, it was assumed that all catalysts would be replaced annually. The limestone requirements were derived from the analyses and data in Reference 38. The resource impact of the electric power consumed would be a function of the mix of powerplants in the utility system, and therefore not specified in more detail in the table.

##### 4.4.4.2 Process Outflows

The products of the process operation, in addition to the hydrogen stream, include a myriad of other flows. The major outflows, on an annual basis, are shown in Table 4.4.5.

##### 4.4.4.3 Process Thermal Efficiency

Thermal efficiency can be expressed in many ways. In Table 4.4.6, it is defined as the higher heating value of the product gas divided by the total heat inputs to the hydrogen generation plant. This includes, of course, not only the energy content of the coal being gasified, but also the energy content of coal and electric power (at an assumed thermal efficiency of about 36 percent) required for the oxygen plant, gas compression to 6895 kPa (1000 psia), and other steam and electric power requirements.

TABLE 4.4.4  
KOPPERS-TOTZEK GASIFICATION  
ANNUAL RESOURCE CONSUMPTION  
(80% Capacity Factor)

Coal	$2.8 \times 10^9$ kg ( $3.1 \times 10^6$ Tons)
Water	$2.0 \times 10^{10}$ kg ( $4.4 \times 10^{10}$ lb)
Electricity	$3.1 \times 10^8$ Kwh
Limestone	$1.1 \times 10^8$ kg (121,000 Tons)
Catalysts and Chemicals	$1.1 \times 10^6$ kg (1250 Tons)

TABLE 4.4.5  
KOPPERS-TOTZEK GASIFICATION  
ANNUAL PROCESS OUTFLOW  
(80% Capacity Factor)

Product Hydrogen Stream	$2.79 \times 10^9$ std/m <sup>3</sup> ( $1.04 \times 10^8$ MSCF)
Waste Streams	
Slag	$2.65 \times 10^8$ kg (292,000 Tons)
Ash (from boilers, etc.)	$1.17 \times 10^8$ kg (129,000 Tons)
Flyash (from boilers, etc. - not recovered)	$6.35 \times 10^5$ kg (700 Tons)
Limestone and Sulfur (flue gas cleanup)	$1.52 \times 10^8$ (167,000 Tons)
Catalysts and Chemicals	$1.1 \times 10^6$ kg (1250 Tons)
CO <sub>2</sub>	$1.85 \times 10^9$ std/m <sup>3</sup> ( $6.9 \times 10^7$ MSCF)
Sulfur-Elemental	$8.16 \times 10^7$ kg (90,000 Tons)

TABLE 4.4.6

KOPPERS-TOTZEK GASIFICATION  
OVERALL PROCESS EFFICIENCY

Heat Inputs

Coal to Gasifiers	7296 GJ/hr (6.92 x 10 <sup>9</sup> Btu/hr)
Other Heat Inputs (coal for steaming, electric power, etc.)	3648 GJ/hr (3.46 x 10 <sup>9</sup> Btu/hr)
<b>Total Heat Input</b>	<b>10,944 GJ/hr (10.38 x 10<sup>9</sup> Btu/hr)</b>

Heat Outputs

Product Gas	3.98 x 10 <sup>5</sup> std m <sup>3</sup> /hr (14.87 x 10 <sup>6</sup> SCF/hr)
Heating Value (weighted)	13.48 MJ /std m <sup>3</sup> (342.5 Btu/SCF)
<b>Total Heat Output</b>	<b>5365 GJ/hr (5.09 x 10<sup>9</sup> Btu/hr)</b>

Overall Efficiency

$$\frac{5365 \text{ GJ/hr} \times 100}{10,944 \text{ GJ/hr}} = 49\%$$

#### 4.4.5 Economics

The cost of producing hydrogen is evaluated for the plant design discussed in Sections 4.4.3 and 4.4.4. In determining the overall costs, estimates were made of the capital, operation and maintenance, and fuel costs for the facility in the general format used in reporting nuclear powerplant costs, as defined in NUS-531 (Reference 32). The effects on the production costs of different capacity factors, coal costs, and type of ownership were also considered.

##### 4.4.5.1 Capital Costs

The capital costs estimate is based on preliminary sizing of most of the major plant equipment and determining appropriate costs for that equipment. Factors, based on experience, were used to account for the costs of installation, piping, valves, instrumentation, structures, and miscellaneous equipment. Indirect costs were also estimated by applying factors as described below.

The plant, producing  $9.56 \times 10^6$  standard  $m^3$ /day ( $356.9 \times 10^6$  SCFD), is estimated to require a direct cost investment, in mid-1974 dollars, of \$260,676,000, as shown in Table 4.4.7. The direct cost accounts are divided among on-sites and off-sites, with the former consisting of closely related mainline processing steps and the latter of support and service systems and facilities. Land is included in the total at an estimated cost of \$1,000,000.

The total plant investment includes the direct costs plus contingencies, indirect costs, and interest during construction. These are shown in Table 4.4.8. For the purpose of evaluation, land and land rights are shown separately from other direct costs since it is a non-depreciating asset.

Special materials comprise the initial supply of chemicals, catalysts, lubricants and other materials needed for operation of the plant. Coal is excluded from this account. A contingency of 15 percent is applied to the estimated cost of the special materials and the direct cost of the physical plant.

Indirect costs are expense items of a general nature which apply to the overall project of building an operable plant, rather than to one of the direct costs. These costs, except for interest during construction, have not been estimated in detail, but calculated as a percentage of the direct costs based on the procedure defined in NUS-531 and up-dated by ERDA in 1974 for use in the study reported in Reference 1.

Construction facilities, equipment, and services include general costs associated with the plant construction, such as field offices, warehouses, temporary power and utility lines, cost or rental of construction equipment and supplies, purchase of electric power, water, and other utilities, security guards, training programs for the labor force, inspection and testing of construction materials, site cleanup, insurance, and the like.

TABLE 4.4.7  
 KOPPERS-TOTZEK GASIFICATION  
 DIRECT CAPITAL COSTS  
 (July, 1974 Dollars)

<u>Account</u>	<u>Item</u>	<u>Installed Cost (\$ Thousands)</u>
<u>2000</u>	<u>On-Sites</u>	
2100	Coal Preparation	\$ 11,556
2200	Coal Gasification	57,348
2300	Acid Gas Removal	6,999
2400	CO Shift	22,062
2500	CO <sub>2</sub> Removal	10,036
2600	Polishing Methanation	3,053
2700	Oxygen Plant	46,440
2800	Sulfur Recovery Plant	4,284
2910	Primary Compression	18,792
2920	Secondary Compression	<u>13,338</u>
	On-Sites Subtotal	\$ 193,908
<u>1000</u>	<u>Off-Sites</u>	
1100	Cooling Towers	\$ 20,098
1200	Make-Up and Feedwater } Effluent Water Treatment	1,085
1300		
1410	Coal Receiving, Storage, Handling	8,714
1420	Slag Disposal	1,630
1430	Flue Gas Clean-Up	10,761
1510	Steam Generation Plant	6,514
1600	Electrical Auxiliary Power	11,185
1700	General Off-Site Investment	
1710	Land and Land Rights	1,000
1720	Site Improvements and Facilities	2,334
1730	Administration/Service Building	734
1740	Instrument and Plant Air	610
1750	Maintenance Facilities	1,293
1760	Fire Protection, Communications	485
1770	Furnishings, Fixtures, Laboratory Equipment	<u>325</u>
	Off-Sites Subtotal	\$ 66,768
	TOTAL DIRECT CAPITAL COST	\$ 260,676



TABLE 4.4.8  
 KOPPERS-TOTZEK GASIFICATION  
 TOTAL PLANT INVESTMENT  
 (In Thousands of Dollars)

<u>Non-Depreciating Assets</u>	<u>Cost</u>
Land and Land Rights	\$ 1,000
<u>Depreciating Assets</u>	
Special Materials	2,992
Physical Plant Direct Cost	<u>259,676</u>
Subtotal	\$ 262,668
Contingency	\$ <u>39,400</u>
Subtotal	\$ 302,068
Indirect Costs	
Constr. Facilities, Equipment, and Services	\$ 17,022
Engineering Services	\$ 25,980
Other Costs	\$ 8,541
Interest During Construction	<u>\$ 52,684</u>
Subtotal	\$ 104,227
Total Depreciating Assets	<u>\$ 406,295</u>
<u>Total Plant Investment</u>	\$ 407,295

Engineering services include items such as preliminary investigations; site selection; air and water environmental studies; subsurface investigations; preparation of specifications and evaluation of proposals for major equipment packages, preparation of preliminary and final design documents, design reviews, procurement, inspection, and expediting of materials and equipment; preparation of pre-operational test and plant startup procedures; assistance in securing plant permits, management and direction of construction activities, including selection of subcontractors, scheduling, maintaining cost and quality control; on-site procurement and receiving of materials and equipment, field accounting, and supervising and pre-operational testing of systems and components; field engineering inspection of construction work to assure compliance with plans and specifications; and preparation of as-built drawings.

Other costs include the owner's property and all-risk insurance, state and local property taxes on the site and improvements during construction, sales taxes on purchased materials and equipment, staff training, plant startup, and the owner's general and administrative (G&A) costs.

Interest during construction is calculated as simple interest, at an 8 percent annual rate, on the plant investment as it is made. For the purpose of the evaluation, it is assumed that the land is purchased six months prior to the start of the project and that special materials are delivered and paid for nine months prior to plant commercial operation. All other plant costs are assumed to accumulate over a six year project period in accordance with Figure 4.4.10. Inherent in this curve is an initial two year period in which expenditures remain low while engineering proceeds, environmental impact statements are prepared, and permits for construction are solicited.

The total plant investment, including all direct and indirect costs, but excluding escalation, is estimated to be \$407,295,000 for the grass roots facility.

#### 4.4.5.2 Operation and Maintenance Costs

The costs of operation and maintenance includes the expense of maintaining a plant staff, consumable supplies and equipment, outside support services, miscellaneous items of cost, and the indirect costs of maintaining the plant working capital.

The direct O&M costs are shown in Table 4.4.9. The staff costs are based on a 180 person staffing level at an average cost of \$19,300 per man-year. The costs of chemicals and catalysts are based on their assumed use rate. A \$300,000 per year allowance has been included for miscellaneous consumables.

An arbitrary allowance of 0.11¢/kg (\$1/Ton) has been provided for the ultimate disposal of solid wastes. This cost must include packaging, transportation, and perpetual storage of all solid wastes from the plant, such as ash and slag, limestone, catalysts, resins, and so forth. Further allowances for contracted work and miscellaneous costs have also been included.

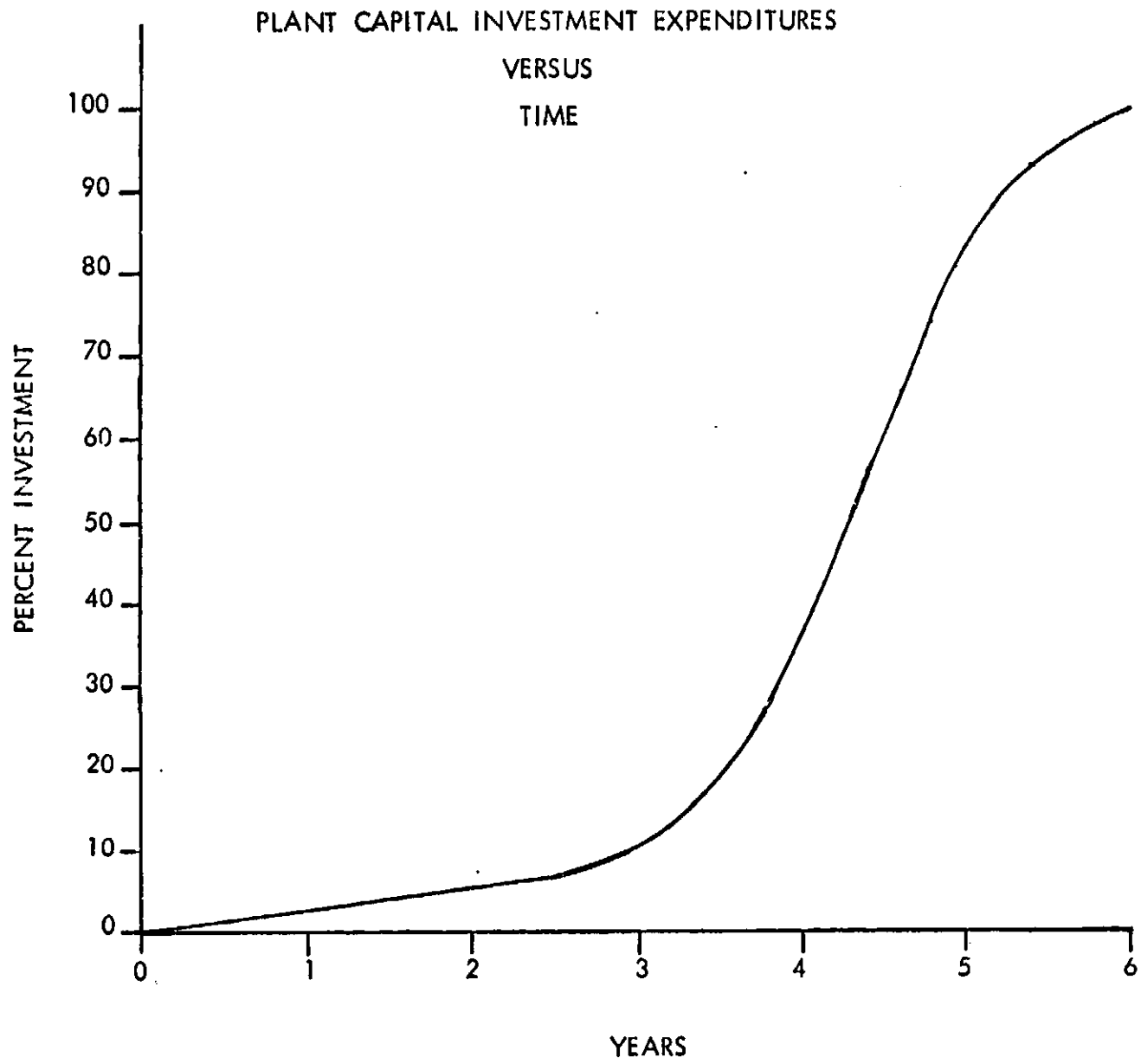


Figure 4.4.10 Coal Gasification

TABLE 4.4.9  
KOPPERS-TOTZEK GASIFICATION  
DIRECT ANNUAL O & M COSTS

<u>Staff Payroll</u>	<u>Costs</u>
180 People	\$ 3,474,000
<u>Consumable Supplies and Equipment</u>	
Chemicals and Catalysts	\$ 3,331,000
Miscellaneous (Lubricants, Maintenance Materials, Filters, Gaskets, Etc.)	<u>300,000</u>
Subtotal	\$ 3,631,000
<u>Outside Support Services</u>	
Ultimate Disposal of Solid Wastes	\$ 637,000
Contracted Work, Consultants, Etc.	<u>140,000</u>
Subtotal	\$ 777,000
<u>Miscellaneous</u>	
Training, Travel, Office Supplies, Etc.	\$ <u>80,000</u>
Subtotal	\$ 7,962,000
<u>G &amp; A</u>	\$ 1,194,000
TOTAL DIRECT O & M COSTS	\$ 9,156,000

The total direct annual operation and maintenance cost of \$9,156,000 includes a 15 percent G&A assessment on the subtotal of all costs.

The indirect O&M costs are shown in Table 4.4.10. These are the costs of maintaining the working capital required for continued operation of the plant and is evaluated at a 10 percent annual charge rate. The working capital is made up of the cash in hand needed to meet the day to day operating expenses plus the value of materials and supplies in inventory. The average net cash required is calculated at 2.7 percent of the direct O&M costs. A two month supply of consumables and coal is assumed to be kept in inventory. The coal is valued, for this purpose, at 2.2¢/kg (\$20/Ton).

The total O&M costs, at a plant capacity factor of 80 percent, are shown in Table 4.4.11.

#### 4.4.5.3 Fuel Costs

Fuel costs, as used here, include the purchase of feedstock and energy, i.e., coal and electric power. For the purpose of a base case calculation, coal, f.o.b. gasification plant site, is assumed to cost 2.2¢/kg (\$20/Ton) and electricity, at an industrial customer rate from the utility system, is costed at 2¢/kwh.

The plant, operating at an 80 percent capacity factor, will consume  $2.8 \times 10^9$  kg/yr ( $3.09 \times 10^6$  tons/year) of coal and  $3.08 \times 10^8$  kwh of electric power, resulting in a total annual "fuel" cost of \$67,983,000.

#### 4.4.5.4 Hydrogen Production Costs

The hydrogen production cost is made up of the contributions of capital, operation and maintenance, and fuel costs. These are normally calculated on an annual basis. The percentage of the plant investment that is charged against production each year is a function of the type of plant ownership, i.e., utility or industrial, and the manner in which the owner can do business. As discussed in Section 4.1.2, the annual charge on non-depreciating assets, e.g., land, is 10 percent for either type of ownership while the annual charge on depreciating assets is 15 percent for utility ownership and 25 percent for industrial ownership. Although production costs are calculated on both a utility and industrial basis, it is not realistic to consider that the production of hydrogen, on the scale contemplated and with distribution to remote "users", would be an "industrial" enterprise. It is considered that this sort of production plant would much more readily fit a "regulated utility" type of enterprise - much like today's natural gas and electric utility operations.

The cost of hydrogen production, on both bases, is shown in Table 4.4.12. As can be seen, the cost, which is equivalent to a "gate selling price", is 5¢/standard m<sup>3</sup> (\$1.34/MSCF), or \$3.71/GJ (\$3.91/10<sup>6</sup> Btu) on a utility basis. The cost to the ultimate consumer would be this production cost plus the allocated capital and operating costs of transmission and distribution.

TABLE 4.4.10  
KOPPERS-TOTZEK GASIFICATION  
INDIRECT OPERATION AND MAINTENANCE COSTS

	<u>Cost</u>
Average Net Cash Required	\$ 247,000
Materials and Supplies in Inventory	
Consumable Supplies and Equipment	\$ 555,000
Coal Storage	\$ 12,702,000
Total Working Capital	\$ 13,504,000
Annual Charge Rate	10%
Annual Indirect O & M Cost	\$ 1,350,000

TABLE 4.4.11  
KOPPERS-TOTZEK GASIFICATION  
TOTAL ANNUAL O & M COST  
(80% Capacity Factor)

	<u>Cost</u>
Direct O & M Costs	\$ 9,156,000
Indirect O & M Costs	\$ <u>1,350,000</u>
TOTAL	\$ 10,506,000

TABLE 4.4.12  
 KOPPERS-TOTZEK GASIFICATION  
 HYDROGEN PRODUCTION COST COMPARISON  
 (80% Capacity Factor)

<u>Annual Costs</u>	<u>Ownership</u>	
	<u>Utility</u>	<u>Industrial</u>
Non-Depreciating Capital	\$ 100,000	\$ 100,000
Depreciating Capital	60,944,000	101,574,000
Operation and Maintenance	10,506,000	10,506,000
"Fuel"	<u>67,983,000</u>	<u>67,983,000</u>
Total Annual Cost	\$139,533,000	\$ 180,163,000
 <u>Annual Gas Production</u>	 2.79 x 10 <sup>9</sup> std m <sup>3</sup> (1.042 x 10 <sup>11</sup> SCF)	 2.79 x 10 <sup>9</sup> std m <sup>3</sup> (1.042 x 10 <sup>11</sup> SCF)
 <u>Production Cost</u>	 \$0.05/std m <sup>3</sup> (\$1.34/MSCF)	 \$0.065/std m <sup>3</sup> (\$1.73/MSCF)
	\$3.71/GJ (\$3.91/10 <sup>6</sup> Btu)	\$4.79/GJ (\$5.05/10 <sup>6</sup> Btu)

#### 4.4.5.5 Sensitivity of Hydrogen Production Costs to Variables

The cost of hydrogen production from any given plant will vary with the cost of feedstocks, the type of ownership, and the utilization, i.e., capacity factor, of the facility. For the base case calculation, it was assumed that coal costs were 2.2¢/kg (\$20/Ton), electricity costs were 2¢/kwh, the capacity factor was 80 percent, and utility ownership prevailed.

Figure 4.4.11 shows the effect on hydrogen production cost of variations in the cost of coal and electric power for both utility and industrial ownership, with the capacity factor remaining at 80 percent as in the base case.

Table 4.4.13 indicates the manner in which the capacity factor affects the production cost. In this table, all of the cost assumptions are the same as the base case with only the capacity factor allowed to vary within a range of 40 to 90 percent. As can be seen, the cost of capital remains constant regardless of how the plant is operated. Operation and maintenance costs are divided into two parts, i.e., fixed and variable. The fixed costs are independent of the plant performance and accrue whether or not the plant is operated. The variable costs are a direct function of the plant operation. Fuel costs are also variable costs.



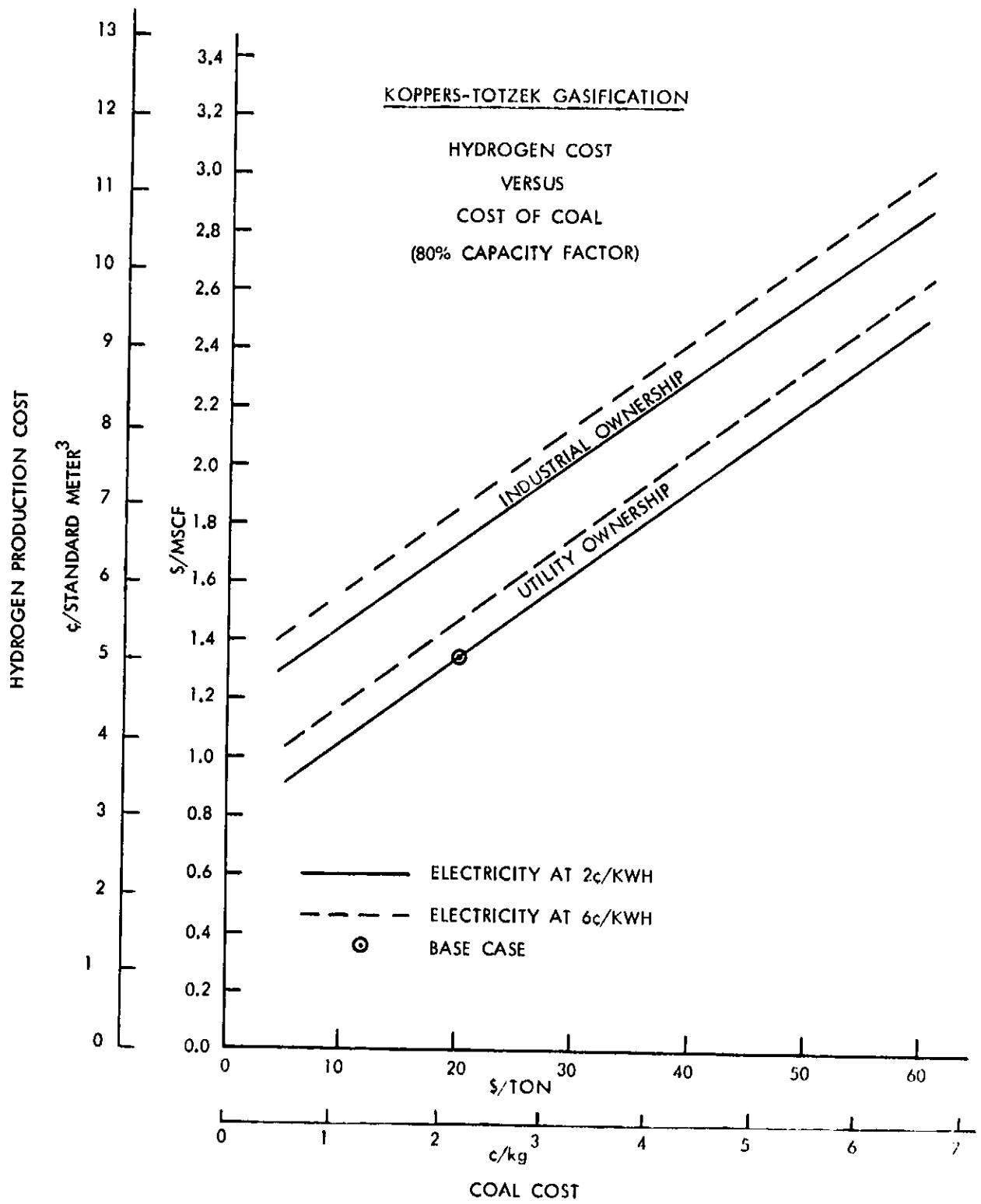


Figure 4.4.11

TABLE 4.4.13

KOPPERS-TOTZEK GASIFICATION  
 SENSITIVITY OF H<sub>2</sub> PRODUCTION COST TO CAPACITY FACTOR  
 (Base Case Cost Assumptions)

Item	<u>Capacity Factor</u>			
	<u>40%</u>	<u>60%</u>	<u>80%</u>	<u>90%</u>
Capital Cost	\$ 61,044,000	\$ 61,044,000	\$ 61,044,000	\$ 61,044,000
Fixed O & M	5,795,000	5,795,000	5,795,000	5,795,000
Variable O & M	2,356,000	3,533,000	4,711,000	5,300,000
Fuel - Coal	30,908,000	46,362,000	61,816,000	69,543,000
Electricity	<u>3,084,000</u>	<u>4,625,000</u>	<u>6,167,000</u>	<u>6,938,000</u>
Total Annual Cost	\$103,187,000	\$121,359,000	\$139,533,000	\$143,620,000
Annual Gas Production	1.40 x 10 <sup>9</sup> std m <sup>3</sup> (5.21 x 10 <sup>10</sup> SCF)	2.09 x 10 <sup>9</sup> std m <sup>3</sup> (7.82 x 10 <sup>10</sup> SCF)	2.79 x 10 <sup>9</sup> std m <sup>3</sup> (1.042 x 10 <sup>11</sup> SCF)	3.14 x 10 <sup>9</sup> std m <sup>3</sup> (1.172 x 10 <sup>11</sup> SCF)
Production Cost	7.37¢/std m <sup>3</sup> (\$1.98/MSCF)	5.81¢/std m <sup>3</sup> (\$1.55/MSCF)	5.00¢/std m <sup>3</sup> (\$1.34/MSCF)	4.73¢/std m <sup>3</sup> (\$1.27/MSCF)

## 4.5 WATER DECOMPOSITION

### 4.5.1 General

The water decomposition system used for hydrogen production is the Westinghouse Sulfur Cycle two-step thermochemical process described in Section 3.4.3. In this process, hydrogen and sulfuric acid are produced electrolytically by the reaction of sulfur dioxide and water. The process is completed by vaporizing the sulfuric acid and thermally reducing, at higher temperatures, the resultant sulfur trioxide into sulfur dioxide and oxygen. Following separation, sulfur dioxide is recycled to the electrolyzer and/oxygen is either vented or sold.

As in conventional water electrolysis, hydrogen is produced at the electrolyzer cathode. Unlike water electrolysis, sulfuric acid, rather than oxygen, is produced at the anode. Operation in this fashion reduces the theoretical power required per unit of hydrogen production by more than 85 percent over that required in water electrolysis. This is partially offset, however, by the need to add thermal energy to the process in the acid vaporizer and the sulfur trioxide reduction reactor. Even so, by avoiding the high overvoltages at the oxygen electrode of a conventional electrolyzer, as well as the inefficiencies associated with power generation, this hydrogen generation process provides overall thermal efficiencies approximately double those attainable by conventional electrolytic hydrogen and oxygen production technology.

The overall process flowsheet for the water decomposition system is shown in Figure 4.5.1. Table 4.5.1 summarizes the nomenclature employed in identifying components of the system.

The energy source for the water decomposition system is a very high temperature nuclear reactor (VHTR) producing both electric power and a high temperature helium stream to the process.

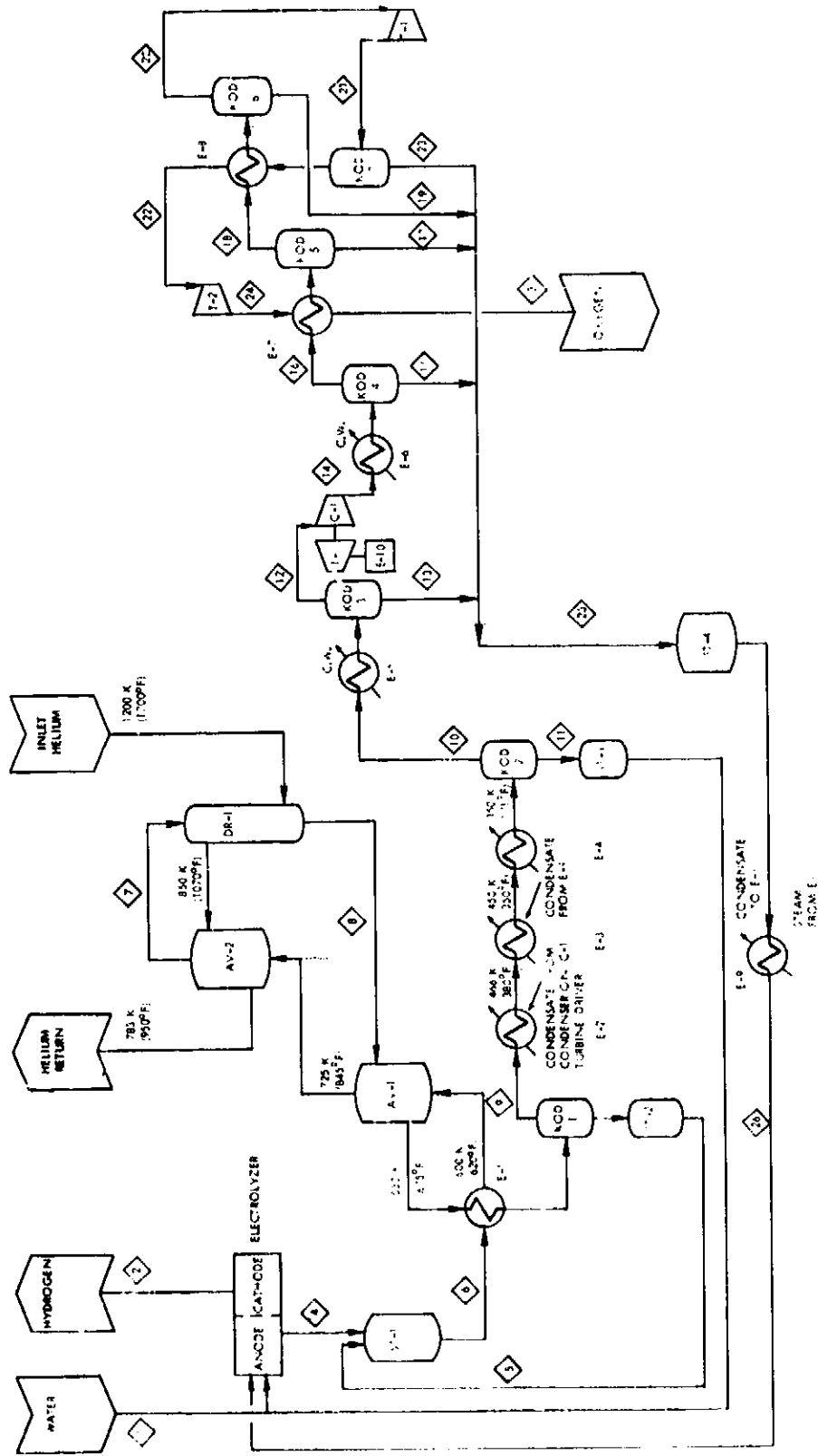
The principal operating and performance characteristics of the water decomposition system are given in Table 4.5.2.

### 4.5.2 Plant Design

In order to provide a basis for cost estimates and evaluation of overall performance, a preliminary conceptual design was prepared. This design is described in the paragraphs below.

#### 4.5.2.1 Plant Layout

The plant is presumed to be located at the Middletown site described in NUS-531 (Reference 32). A preliminary plot plan was prepared, showing the general location and space requirements for all plant facilities, including the nuclear heat source. This is shown



STREAM	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
TEMPERATURE (K)																
TEMPERATURE (°F)																
PRESSURE (PSIA)																
MASS FLOW RATE (lb/min)																
ENTHALPY (Btu/lb)																
ENTHALPY (Btu/min)																
ENTHALPY (Btu/hr)																
ENTHALPY (Btu/sec)																
ENTHALPY (Btu/min)																
ENTHALPY (Btu/hr)																
ENTHALPY (Btu/sec)																
ENTHALPY (Btu/min)																
ENTHALPY (Btu/hr)																
ENTHALPY (Btu/sec)																

Figure 4.5.1 Westinghouse Hydrogen Generation Process Flowsheet

TABLE 4.5.1  
COMPONENT NOMENCLATURE

AV-1, AV-2	Feed Acid Vaporizers
C-1	SO <sub>2</sub> /O <sub>2</sub> Compressor
DR-1	SO <sub>3</sub> Reduction Reactor
E-1	Feed Acid Preheater/ Recycle Acid Condenser
E-2	Steam Generator for C-1 Turbine Drive
E-3	Steam Generator for SO <sub>2</sub> Vaporizer
E-4	Recycle Water Condenser
E-5	SO <sub>2</sub> Condenser
E-6	SO <sub>2</sub> Condenser
E-7, E-8	Gas Intercoolers
E-9	SO <sub>2</sub> Vaporizer
E-10	Turbine Drive Condenser
KOD-1	Recycle Acid Knockout Drum
KOD-2	Recycle Water Knockout Drum
KOD-3 to KOD-7	Recycle SO <sub>2</sub> Knockout Drums
ST-1	Feed Acid Surge Tank
ST-2	Recycle Acid Surge Tank
ST-3	Recycle Water Surge Tank
ST-4	SO <sub>2</sub> Surge Tank
T-1, T-2	Oxygen Turboexpanders
T-3	Compressor Turbine Drive

TABLE 4.5.2

PRINCIPAL OPERATING AND PERFORMANCE CHARACTERISTICS OF THE  
WESTINGHOUSE SULFUR CYCLE WATER DECOMPOSITION SYSTEM

General

Hydrogen Production Rate	$10.09 \times 10^6$ std m <sup>3</sup> /day	( $379 \times 10^6$ SCFD)
Hydrogen Purity	99.9 volume percent	
Oxygen Production Rate	305,500 kg/hr	(673,000 lb/hr)
Nuclear Heat Source Rating	3220 MWt	
Net Process Thermal Efficiency	47 percent	

Electrolysis

Acid Concentration	80 wt percent	
Pressure	2586 kPa	(375 psia)
Temperature	361 K	(190°F)
Electrolyzer Power Req't	482 MWe	
Cell Voltage, Nominal	0.48 volts	
Cell Current Density, Nominal	2000 A/m <sup>2</sup>	(186 A/ft <sup>2</sup> )

Sulfur Trioxide Reduction System

Peak Temperature	1144K	(1600°F)
Operating Pressure	2068 kPa	(300 psia)

Sulfur Dioxide - Oxygen Separator System

SO <sub>2</sub> Liquefaction Pressure	5171 kPa	(750 psia)
Oxygen Discharge Pressure	517 kPa	( 75 psia)

in Figure 4.5.2 The facilities associated with the plant are grouped in the categories of the VHTR (nuclear heat source), the H<sub>2</sub> plant on-sites, and the support facilities, or off-sites. Within each category, "batteries", identified by an alphabetic or alpha-numeric designation, are defined. These batteries are used to describe related groups of equipment for both design and cost estimating purposes.

#### 4.5.2.2 The Very High Temperature Reactor (VHTR)

The very high temperature nuclear reactor (VHTR), suitable for use with the water decomposition system, is predicated on the integration of the technologies from the NERVA nuclear rocket engine program and land based gas cooled reactor programs into an advanced graphite moderated, helium cooled reactor. The VHTR conceptual design, costs, and R&D program required for demonstration are more fully described in Reference 1. The plant consists of a Nuclear Island producing both high temperature heat and electric power for the chemical water decomposition process. The heat is transported to the process via an intermediate heat transfer loop at temperatures sufficiently high to permit peak process temperatures of 1144K (1600°F).

The reactor and its coolant loops are contained within a multi-cavity prestressed cast iron reactor vessel (PCIV), as shown in Figure 4.5.3. The vessel walls contain smaller vertical cavities, or pods, in which are high temperature intermediate heat exchangers, circulators, turbogenerators and low temperature intermediate heat exchangers or auxiliary cooling systems for shutdown and emergency cooling of the reactor. Reactor helium coolant enters and discharges from the pods through coaxial piping at the upper end of the cavity, while the intermediate loop, or secondary, helium coolant is introduced and leaves through the bottom of the pod. The PCIV has a continuous internal steel liner to act as a primary coolant boundary and leak tight membrane. A thermal barrier and insulation system is used to limit the temperature of the liner and minimize the heat loss to the PCIV. A cooling system circulates water through the walls of the PCIV to remove the heat deposited in the vessel. The PCIV is fabricated as a series of foundry cast iron blocks field assembled around the welded steel liner. Prestress cables are wound around the external cylindrical surface, imposing a high compressive stress on the vessel assembly in the radial and tangential directions and preventing the castings from separating under the internal gas pressure forces. Similarly, axial cables running longitudinally, through ports provided in the castings, maintain a high compressive stress in the axial direction and carry the axial pressure loads.

The reactor core is designed to operate on the U-235/thorium-232 cycle. The basic concept of fuel moderator blocks for the reactor is similar to that used in other gas cooled reactors. The extruded fuel elements are directly cooled by the helium.

An objective in the core thermal design is to use an existing fuel particle, i.e., the TRISO bead, in the fissile fuel element and to achieve a high exit gas temperature without exceeding the fuel particle limitations.

**H<sub>2</sub> PROCESS PLOT PLAN**

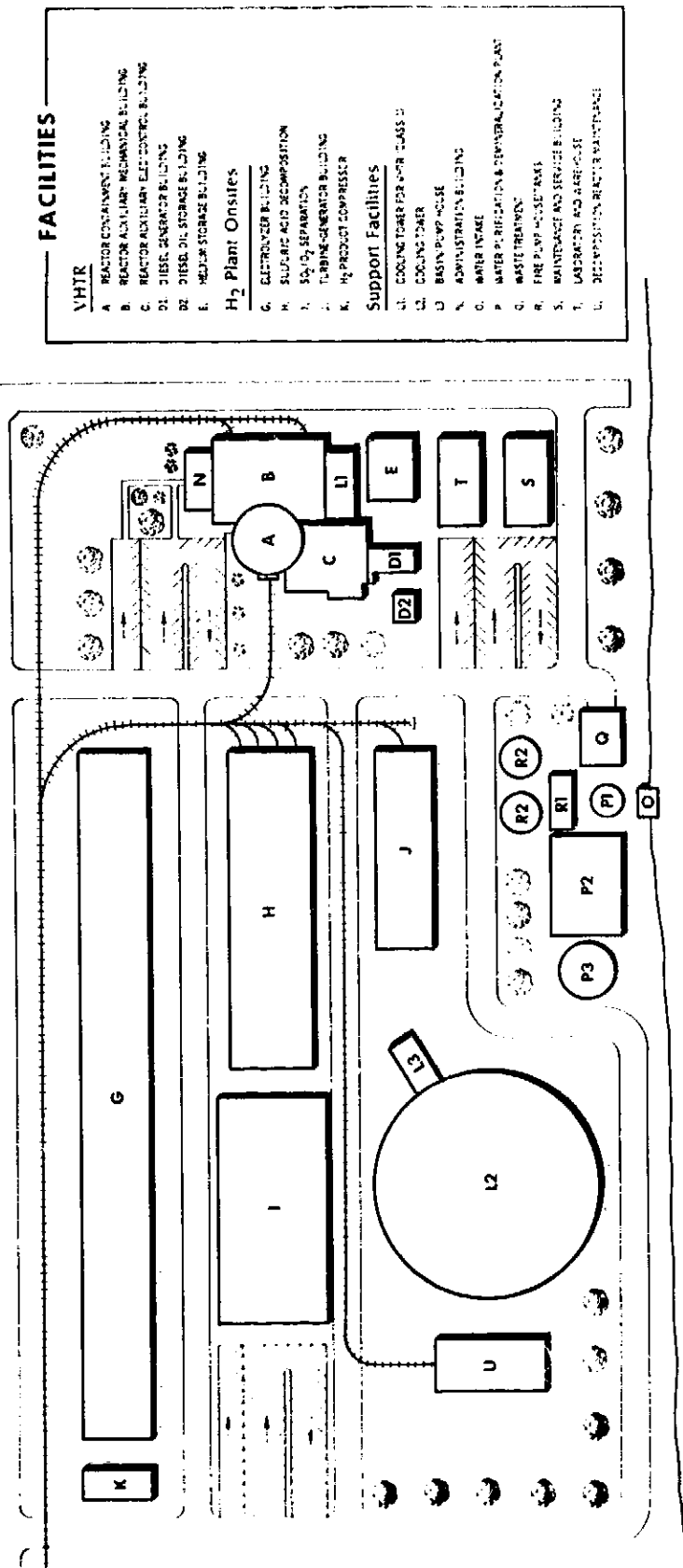


Figure 4.5.2 Westinghouse Process Plot Plan



# VHTR FOR PROCESS HEAT

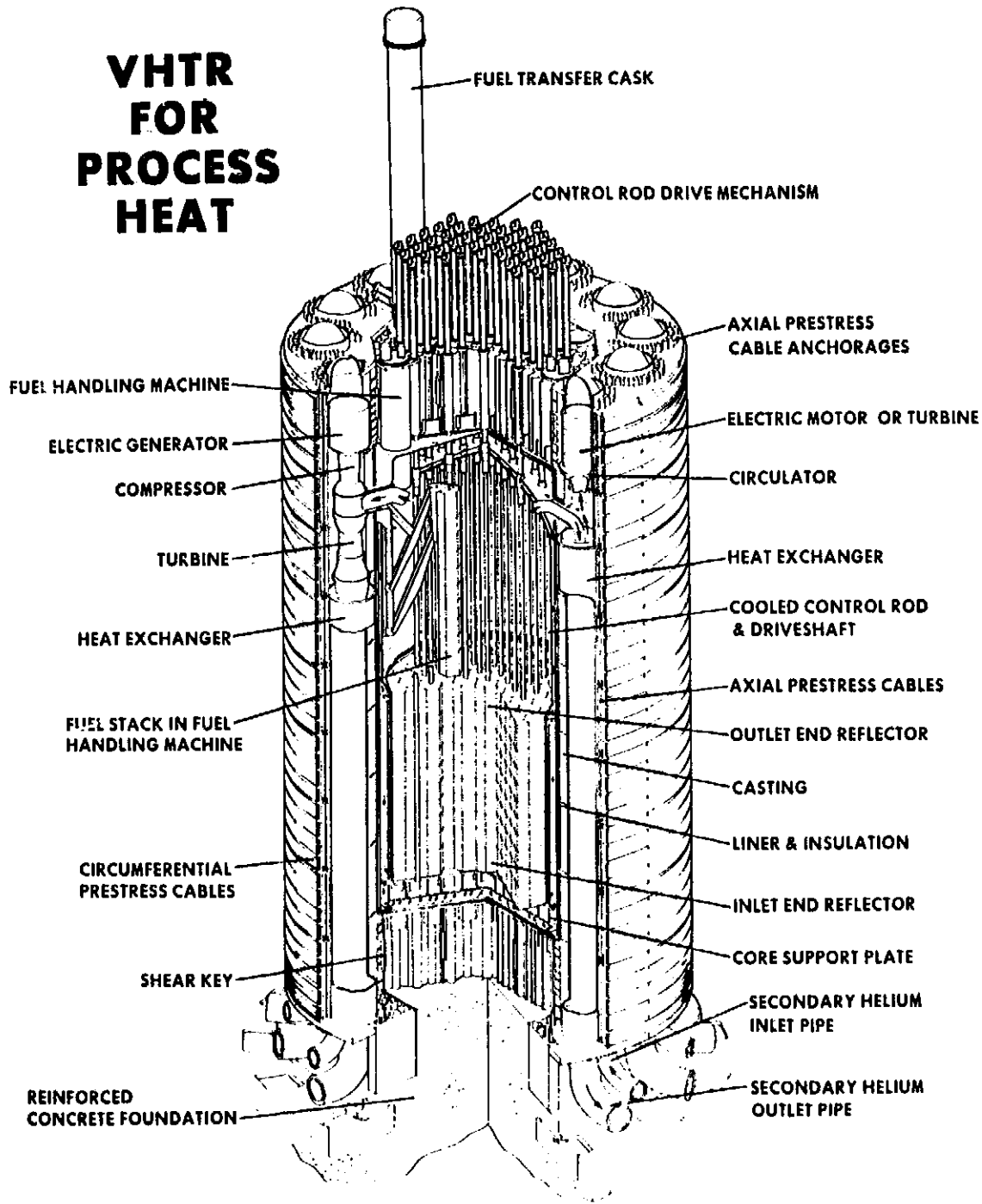


Figure 4.5.3 Very High Temperature Reactor (VHTR)

The reactor coolant system consists of the parallel power and heat exchanger loops located in the PCIV cavities. The function of the high temperature intermediate heat exchange loops is to transfer heat from the reactor core to the intermediate helium loops, which in turn transfer this heat to the high temperature  $\text{SO}_3$  reduction reactor. Each loop contains a high temperature heat exchanger, valve, and helium circulator. The turbogenerator loops generate electric power and supply lower temperature heat, via low temperature intermediate heat exchangers, to steam generators in Battery J for the production of additional electric power in a Rankine cycle. Principal parameters of the reactor are shown in Table 4.5.3.

Associated with the reactor are all the ancillary structures, services, systems, and facilities to make a self-sufficient, operable Nuclear Island. These include reactor auxiliary systems, waste processing systems, instrumentation and control, fuel handling facilities, containment systems, electrical systems, and plant service systems.

### Major Features

A number of significant features have been incorporated into the conceptual design of the very high temperature reactor (VHTR) to make it particularly attractive as a heat source for the water decomposition system.

Fuel. The ability to achieve the very high temperatures needed for the application, without exceeding the fuel bead temperatures currently considered as maximum allowable, is achieved with extruded direct cooled fuel elements.

Reactor Vessel. Three different reactor vessel types had been considered. These were a welded steel vessel, a prestressed concrete vessel (PCRV) and a prestressed cast iron vessel (PCIV).

The steel vessel was discarded on the basis of the problems foreseen in the manufacture and transportation of vessels of the size required for large gas cooled reactors. The alternate of a field assembled welded steel vessel would require a very complex "one-time" fabrication facility and quality assurance program. The prestressed concrete reactor vessel (PCRV) technology has been used in European gas cooled reactors and is currently being applied in the United States. There does not appear to be any reason why the reactor could not be accommodated in a PCRV.

The prestressed cast iron reactor vessel (PCIV) design is based on analytical and experimental work by the German firm, Siempelkamp Giesserei AG, Krefeld, West Germany. The concept is generally similar to that of the PCRV, with the exception that the concrete is replaced by cast iron. Cast iron compressive strength is twenty times that of concrete while its density and Young's Modulus are three times that of concrete. In addition, it has predictable physical properties and little or no in situ creep or shrinkage. It has reduced weight and size, see Table 4.5.4, with reduced sensitivity to overtemperature incidents. The cast iron blocks are poured and machined under factory, rather than field, conditions,

TABLE 4.5.3  
PRINCIPAL PARAMETERS OF THE VHTR

Reactor Thermal Power, MWT	3220
Reactor Vessel	
Type	Prestressed Cast Iron
Overall Height, Meters (ft)	33.5 (110)
Overall Diameter, Meters (ft)	20.1 (66)
Material	Gray Iron (Class 40)
Reactor Core	
Nominal System Pressure, kPa (psia)	6895 (1000)
Coolant Mixed Mean Outlet Temperature, K (°F)	1283 (1850)
Reactor Power Density, W/cm <sup>3</sup>	10
High Temperature Intermediate Heat Exchangers	
Coolant, Tube Side/Shell Side	Helium/Helium
Pressure, Tube Side/Shell Side, kPa	6895/6895
Intermediate Coolant Outlet Temperature, K (°F)	1200 (1700)
Circulators	
Type	Axial Flow
Inlet Pressure, kPa (psia)	6688 (970)
Discharge Pressure, kPa (psia)	6895 (1000)
Turbogenerators	
Turbine Inlet Temperature, K (°F)	1283 (1850)
Electric Power Output, MW	231
Low Temperature Intermediate Heat Exchanger	
Coolant, Tube Side/Shell Side	Helium/Helium
Intermediate Coolant Outlet Temperature, K (°F)	929 (1212)

TABLE 4.5.4  
REACTOR VESSEL COMPARISON

	<u>Prestressed Cast Iron (PCIV)</u>	<u>Prestressed Concrete (PCRV)</u>
Overall Height, meters	33.5	39.6
Overall Diameter, meters	20.1	32.9
Wall Thickness, meters	4.3	10.7
Head Thickness, meters	4.0	7.3

resulting in a greater capability for the control of quality. Other foreseeable advantages include reduced construction time, reduced reactor containment building size, and reduced cost.

Reactor Flowpath. It is especially desirable, as coolant temperature is increased, to devise design solutions which minimize the problems of materials, insulation, and fabrication. The proper choice of coolant flowpath is important to the design of the reactor vessel, liner, control rods, and drive mechanisms. The selected approach is to use the low temperature helium, returning to the reactor, to cool those components that would otherwise be exposed at or near the reactor exit gas temperatures of 1283K (1850°F).

Parallel Gas Turbine and High Temperature Process Heat Loops. The energy requirements of a process are, in general, heat at several temperature levels and electric power in varying amounts depending upon the process configuration. To most effectively meet these energy needs, an arrangement of parallel electric power and process heat loops has been adopted.

Intermediate Loop. When considering the use of nuclear heat in a process plant, the question of how that heat is to be applied must be answered. There are two alternatives, i.e., the direct cycle, where the reactor coolant is used in the process heat exchanger, and the indirect or intermediate loop cycle, where the reactor coolant transfers its heat to an intermediate buffer coolant system which in turn gives us its heat in the process heat exchanger.

The choice of the intermediate heat transfer loop approach for the process heat reactor was made after considering the advantages and disadvantages of the two alternatives in light of the all-important criteria of operability, maintainability, licenseability, and economics. The cost of additional equipment and higher reactor coolant temperatures must be balanced against the other factors of operation and maintenance procedures and costs, licensing requirements, and public acceptance.

### Reactor Core

The reactor core is characterized by a large volume, large inventory of fertile material with its attendant prompt negative coefficient of reactivity and low power density. The reactor fuel takes advantage of the unique capability of ceramic fuel microspheres to achieve very high burnups. Low temperature gradients in the extruded fuel elements are expected to minimize the adverse effects of temperature gradients on the integrity of fuel beads (the amoeba effect).

The flexibility of the core design facilitates the consideration of alternative fuel configurations, coolant control schemes and refueling cycles.

The reactor core consists of sixty-one columns, each composed of eight hexagonal moderator blocks and one reflector block at each end of the core. Each moderator block has two types of fuel — fissile (highly enriched U-235) and fertile (natural thorium) on a one-to-two ratio, respectively. A central hole is incorporated in each moderator block to allow for the passage of the control rod and fuel handling tools.

### Reactor Coolant System

The reactor coolant system consists of the high temperature heat exchanger loops, the turbocompressor generator loops, the auxiliary cooling loops and the structures and ducting required to direct the cooling flow through the reactor and loops.

The reactor coolant is helium, which is chemically inert, is stable, is not subject to phase change and has excellent heat transfer characteristics. Helium has essentially zero neutron capture cross section, except for the fraction of helium-3 present in the gas. Some impurities will be present in the primary coolant due to desorption of impurities from material in the primary system, due to residual air during initial plant startup and release of gaseous fission products. The release of gaseous fission products is the only significant source that affects the steady state impurity level, and this concentration will be small due to the small mass of gaseous products produced by the fission process and the ability of the coated fuel particles to retain fission products.

The function of the turbocompressor loops is to generate electrical power and supply relatively low temperature heat energy. These loops contain gas turbines, low temperature heat exchangers, valves and compressors.

There are two auxiliary cooling loops to provide independent means of cooling the reactor system when the reactor is shut down. The major components included in the auxiliary cooling loops are heat exchangers, shutoff valves, and circulators.

Gas Circulators. Each of the intermediate heat exchanger loops is provided with its own gas circulator. To permit the necessary independence and capability to handle each IHX pod as a separate unit, these circulators are powered by individual electric motor drives.

Intermediate Heat Exchanger. The principal requirements for heat exchangers, in this application, are the high temperature intermediate heat exchanger, the low-temperature intermediate heat exchanger, and the SO<sub>3</sub> reduction reactor. These heat exchangers must operate for long periods of time under high temperature conditions, while maintaining a high degree of leak tightness. The intermediate heat exchangers also have to meet the requirements of the nuclear codes. The process heat exchanger (DR-1), must handle similar temperatures while operating in the chemical environment of the water decomposition process.

Material limitations become the constraining factor in high temperature heat exchanger designs. It is believed possible to obtain the 1144K (1600°F) process temperature within the limits of the capability of present superalloys that can be applied in the intermediate and process heat exchangers.

#### 4.5.2.3 Battery G - Electrolyzer

The electrolyzers are located in a separate building, identified as G on the plot plan, along with their associated equipment and service facilities. These are a total of 480 electrolyzer modules, each rated at 1 MWe, 100 V-dc, 10,000 amperes.

Rectifiers are employed to supply the dc power to the electrolyzers. Each Rectifier, rated at 24 MWe, 2400 V-dc, 10,000 amperes feeds 24 electrolyzers in series. The Rectifier consists of an a-c connection (3 phase, 60 hz), regulating transformer, stepdown transformer, diodes (rectifiers), and a d-c connection. Controls are supplied to vary the a-c voltage to adjust the d-c voltage for changes in the electrolyzer module circuits, such as a module taken out of service. The Rectifiers are located outside the electrolyzer building.

Surge tanks (ST-1) associated with the collection of sulfuric acid from the electrolyzers, are also located outside the electrolyzer building. The characteristics of the surge tank is shown in Table 4.5.5.

The electrolyzer building is of steel siding and roofing on a concrete slab. The building is 305 meters (1000 feet) long by 36.6 meters (120 feet) wide by 8.5 meters (28 feet) from the top of the floor slab to the roof siding eave line. A double ridge roof is provided with ventilators running the length of the building in each ridge to assure free and rapid escape of buoyant hydrogen from the building in the unexpected event of a hydrogen line rupture.

TABLE 4.5.5

## ELECTROLYZER SURGE TANK (ST-1) CHARACTERISTICS

Number of Tanks	20
Tank Outside Diameter	2.44 meters (8 feet)
Total Tank Length	6.4 meters (21 feet)
Normal Operating Pressure	2586 kPa (375 psia)
Normal Operating Temperature	433K (320°F)
Material of Construction	Hastelloy . C
Process Fluid	80 wt % H <sub>2</sub> SO <sub>4</sub>

4.5.2.4 Battery H - Sulfuric Acid Decomposition

The sulfuric acid decomposition battery consists of that equipment required to take the 80 wt percent sulfuric acid from the electrolyzer, vaporize it, decompose it to water and sulfur trioxide, and reduce the sulfur trioxide to sulfur dioxide and oxygen. The equipment required for these functions are all housed in one building, identified by the letter "H" on the plot plan.

The components of this battery are the Feed Acid Preheater/Recycle Acid Condenser (E-1), the recuperatively heated Feed Acid Vaporizer (AV-1), the helium heated Feed Acid Vaporizer (AV-2), and the Sulfur Trioxide Thermal Reduction Reactor (DR-1). Process conditions for the components are shown in the overall flowsheet, Figure 4.5.1.

The operating pressures and temperatures selected for the initial design result in materials requirements, for E-1, AV-1, and AV-2, that are beyond today's industrial experience in handling boiling and condensing sulfuric acid. These heat exchangers, therefore, must employ materials for which corrosion data, at the operating conditions, do not exist. Potential materials that might be applicable include Hastelloy C, Incolloy 625, or some metallic alloy with a vapor phase deposited silicon coating. Development work is required to determine what materials can ultimately meet these conditions. Section 5 discusses in more detail the consideration of structural materials for this service.

Alternate operating parameters and process configurations for the sulfuric acid decomposition system can be considered which will permit design conditions much closer to the temperatures at which material data is available. The current flowsheet calls for operation of the process at 2068 kPa (300 PSIA), requiring vaporization of sulfuric acid at a temperature of about 725K (845°F) approximately 110 to 170K (200 to 300°F) above the temperatures at which extensive corrosion data is available.

Reducing the process pressure to 172 to 517 kPa (25 to 75 psia) permits consideration of high silicon irons, such as Duriron. Material fabrication difficulties, however, must be examined. Current technology is limited to roughly 2.54 cm (one inch) tubes in 0.9 meter (three foot) lengths. Development effort would be required to produce longer tube and shell heat exchangers. Duriron can be fabricated into approximately 1.2 m (4 feet) by 1.8 m (6 feet) sheets, however, introducing the possibility of using plate heat exchangers for the sulfuric acid vaporizers.

The configuration of the recuperative heat exchange system can also be changed. The current flowsheet employs exchangers E-1 and AV-1 to affect feed acid preheat and vaporization using heat from condensing unreacted sulfuric acid present in the effluent from the thermal reduction reactor DR-1. This recuperative heat exchange can be accomplished in several ways. One possible alternate considers acid from the electrolyzer surge tank being injected into the high temperature effluent from the thermal reduction reactor. This provides a rapid quench, lowering the temperature of the gas to a nominal value of about 644K (700°F). This cool gas is then passed through a ceramic lined and packed tower, irrigated with additional electrolyzer acid. Leaving the tower is a wet SO<sub>2</sub>/O<sub>2</sub> stream and condensed acid for recycle to the helium heated vaporizer (AV-2). The use of this type of recuperative heat exchange system reduces by over 50 percent the heat transfer surface required to withstand corrosive service.

These alternates will be considered as part of the conceptual design to be prepared in Task III (to be reported separately).

The specific design of the Sulfur Trioxide Thermal Reduction Reactor (DR-1) is to be prepared as part of the Task III effort. In order to be able to specify a realistic design, Westinghouse has been conducting an experimental program to evaluate potential catalysts for use in the reactor. Kinetic data obtained over selected catalysts have been analyzed and the reaction order determined. The rate constants are Arrhenius, and the pre-experimental constants as well as the activation energies have been calculated from the data.

Catalysts with sufficient activity to permit compact reduction reactors have been identified and are presently undergoing life testing. One such catalyst has operated at 1125K (1565°F) and a space velocity of 30,000 hr<sup>-1</sup> for long periods of time without any discernible loss of activity.



Using catalyst activity information of this type, preliminary designs of the sulfur trioxide thermal reduction reactor are being prepared. Two arrangements are being considered, depending upon whether one or two reduction catalysts are used. The use of a single catalyst possessing high activity over the entire temperature range leads to a process configuration employing a single reduction reactor in each of five parallel process trains. Alternatively, if two catalysts are used - one possessing good low temperature activity and the second possessing good high temperature activity - a five by two arrangement would be used.

Table 4.5.6 shows the principal characteristics of the components of the sulfuric acid decomposition system.

#### 4.5.2.5 Battery I - SO<sub>2</sub>/O<sub>2</sub> Separation

The SO<sub>2</sub>/O<sub>2</sub> separation system handles the effluent from the sulfuric acid decomposition system, as shown in Figure 4.5.1. A stream of gas and unreacted sulfur trioxide, from E-1, is fed to a knock-out system (KOD-1), where the SO<sub>3</sub> is recovered as sulfuric acid and returned to the sulfuric acid decomposition system. Wet sulfur dioxide and oxygen flow to the separation system. Steam is first condensed, following which the SO<sub>2</sub>/O<sub>2</sub> mixture is compressed to 5171 kPa (750 psia) and sulfur dioxide recovery is affected.

Bulk sulfur dioxide removal is accomplished by condensation against cooling water. Final removal is achieved by condensation against low-temperature oxygen. This refrigeration and some auxiliary power production is generated by the expansion of the oxygen stream prior to its venting.

The characteristics of the major equipment in Battery I are shown in Tables 4.5.7 and 4.5.8. Table 4.5.7 describes heat exchangers in the system while Table 4.5.8 presents information on surge tanks and knock-out drums.

Compressor C-1 is a steam turbine driven three stage centrifugal compressor raising the pressure of 305,500 kg/hr (673,500 lb/hr) of oxygen and 239,000 kg/hr (527,000 lb/hr) of sulfur dioxide from 2069 kPa (300 psia) to 5171 kPa (750 psia).

Turboexpanders T-1 and T-2 are used to reduce the oxygen pressure from 5171 kPa (750 psia) to 2068 kPa (300 psia), and 2068 kPa (300 psia) to 517 kPa (75 psia), respectively, with the recovery of about 4250 kw of power in the process.

#### 4.5.2.6 Battery J - Turbine-Generator

Electric power for use in the hydrogen production plant is generated from several sources. The bulk of the power is generated by a combined Brayton-Rankine cycle with a total generating capacity of approximately 581,000 kw. This power is distributed within the plant to provide about 480,000 kw for the hydrogen-producing electrolyzers and the remainder for operation of equipment within both the nuclear heat source (VHTR) and the hydrogen generation plant.

TABLE 4.5.6

## SULFURIC ACID DECOMPOSITION COMPONENTS

Component	E-1	AV-1	AV-2	DR-1
Number of Units	5	5	8	5
Characteristic Per Unit				
Heat Duty - MW	58.6	223	128	196
- Btu hr	$200 \times 10^6$	$763 \times 10^6$	$437 \times 10^6$	$669 \times 10^6$
Surface Area - m <sup>2</sup>	725	3530	4180	(1)
- ft <sup>2</sup>	7,800	38,000	45,000	(1)
Pressure, Tube Shell - kPa	2068/2068	2068/2068	6895/2068	6895/2068
- psi	300/300	300/300	1000/300	1000/300
Inlet Temperature, Tube/Shell - K	530/433	1144/600	850/725	1200/725
- °F	675/320	1600/620	1070/845	1700/845
Outlet Temperature, Tube Shell - K	570/600	530/725	783/725	850/1144
- °F	567/620	675/945	950/345	1070/1600
Overall Diameter - m	1.55	3.35	3.66	(1)
- ft	5.1	11.0	12.0	(1)
Overall Length - m	7.92	7.92	7.92	(1)
- ft	26	26	26	(1)

Specific Design to be Determined as Part of Task III. See Text.

TABLE 4.5.7

HEAT EXCHANGERS - SO<sub>2</sub>/O<sub>2</sub> SEPARATION

Component	E-2	E-3	E-4	E-5	E-6	E-7	E-8	E-9	E-10
Number of Units	5	5	6	5	3	3	3	8	2
Characteristics Per Unit									
Heat Duty - MW	14.9	24.0	37.8	8.49	2.05	3.51	2.64	14.9	23.1
Btu/hr	51 x 10 <sup>6</sup>	82 x 10 <sup>6</sup>	129 x 10 <sup>6</sup>	29 x 10 <sup>6</sup>	7 x 10 <sup>6</sup>	12 x 10 <sup>6</sup>	9 x 10 <sup>6</sup>	51 x 10 <sup>6</sup>	79 x 10 <sup>6</sup>
Surface Area - m <sup>2</sup>	2810	613	1700	752	362	873	836	3710	2040
ft <sup>2</sup>	30,200	6,600	18,300	8,100	3,900	9,400	9,000	39,900	22,000
Pressure, Tube Shell - kPa	1034/2068	2068/414	2068/483	2068/103	5171/103	5171/517	5171/2068	2586/414	103/103
psi	150/300	300/60	300/70	300/15	750/15	750/75	750/300	375/60	15/15
Inlet Temperature, Tube Shell - K	510/333	466/419	450/305	350/305	378/305	311/159	266/144	308/419	305/373
°F	567/212	380/294	350/90	171/90	220/90	100/-173	20/-200	94/294	90/212
Outlet Temperature, Tube Shell - K	466/422	450/419	350/328	311/328	311/328	266/295	200/244	370/419	328/373
°F	380/300	350/294	171/130	100/130	100/130	20/72	-100/-20	206/294	130/212
General Diameter - m	3.05	1.43	2.38	1.58	1.52	1.71	1.68	3.51	2.62
ft	10.0	4.7	7.8	5.2	5.0	5.6	5.5	11.5	8.6
Outlet Length - m	7.92	7.92	7.92	7.92	3.96	7.92	7.92	7.92	7.92
ft	26.0	26.0	26.0	13.0	26.0	26.0	26.0	26.0	26.0

TABLE 4.5.8

SURGE TANKS AND KNOCK-OUT DRUMS - SO<sub>2</sub>/O<sub>2</sub> SEPARATION

Component	ST-2	ST-3	ST-4	KOD-1	KOD-2	KOD-3	KOD-4	KOD-5	KOD-6	KOD-7
Number of Units	5	5	5	5	5	3	3	3	3	3
Outside Diameter - m	2.44	2.44	2.44	3.35	2.44	1.83	1.22	1.22	1.22	1.22
- ft	8	8	8	4	8	6	4	4	4	4
Overall Length - m	6.40	6.40	6.40	3.35	2.44	1.83	1.83	1.83	1.83	1.83
- ft	21.0	21.0	21.0	11.0	8.0	6.0	6.0	6.0	6.0	6.0
Nominal Operating Pressure - kPa	2586	2068	2068	2068	2068	2068	5171	517	5171	2068
- psi	375	300	300	300	300	300	750	75	750	300
Nominal Operating Temperature - K	570	350	308	570	350	311	311	266	200	144
- °F	567	171	94	567	171	100	100	20	-100	-200
Material of Construction	Hastelloy	C.S.	C.S.	Hastelloy	C.S.	C.S.	C.S.	C.S.	304 SS	304 SS

The helium Brayton cycle gas turbomachinery, within the VHTR, operating at a gas inlet temperature of 1283K (1850°F) produces an electrical output of approximately 231,000 kw. The "waste" heat from this equipment is transferred, through a low temperature intermediate heat exchanger to an intermediate helium heat transport system. The intermediate helium coolant is used to produce steam, in two parallel generators at a pressure of 10,340 kPa (1500 psia) and 811K (1000°F). The steam is fed to a tandem compound condensing 3600 rpm turbogenerator, exhausting at 17.9 kPa (5.3 inch Hg abs), to produce approximately 350,000 KWe.

The turbine generator building, measuring 76.2 m (250 ft) by 30.5 m (100 ft) by 32.3 m (106 ft) high, houses all of the mechanical equipment, including the intermediate heat transport loop helium circulators, required to extract the sensible heat from the hot helium, convert this energy into steam to drive a turbine-generator set, and condense the exhaust steam into liquid water to start the cycle again.

#### 4.5.2.7 Battery K - Hydrogen Product Compressors

In accordance with the groundrule for the plant design that the product gas must be suitable for pipeline transmission, a compressor station is included in the plant complex to compress the hydrogen gas from its generation pressure of 2586 kPa (375 psia) to 6895 kPa (1000 psia). This is done with four heavy duty seven throw, single stage reciprocating compressors. Power for the compressors is provided by 5220 kW (7000 hp) motors.

#### 4.5.2.8 Cooling Water System

To minimize thermal discharges to the river, a wet mechanical draft cooling tower is used for ultimate heat rejection. This tower, 122 meters (400 ft) in diameter, has twelve fans rated at 149 kW (200 hp) each. The tower has a height of 12.2 m (40 ft) from the top of the basin to the top of the fan deck. The fan cylinders add 5.8 m (19 ft) to the overall height. The tower has the capacity to dissipate approximately 1046 MWt ( $48 \times 10^8$  Btu/hr) of heat.

Four 1492 kw (2000 hp) circulating water pumps are installed in a structure adjacent to the cooling tower basin.

#### 4.5.2.9 Water Make-Up and Waste Treatment Systems

The water requirements for the plant are met by a make-up system taking suction from the river. A pump house, located at the river, contains the raw water pumps and the trash rakes and traveling screens needed to keep the make-up water free from debris.

The raw water is pretreated by a clarifier (coagulator) and filters to make it suitable as feed to the fire protection system, sanitary system, general plant services, and the make-up demineralization system. The pretreatment system has a nominal capacity of 11.36 m<sup>3</sup>/min (3000 gpm).

The clarified and filtered water, to be demineralized, flows initially through a cation exchanger where calcium, magnesium, sodium, and other cations that might be present are exchanged for an equivalent amount of hydrogen ions. The de-cationized water then passed through a forced draft type degasifier where dissolved carbon dioxide is removed to a low level. The degasified effluent then flows through an anion exchanger to remove chloride, sulfate, and other anions. The effluent from the anion exchanger flows through a mixed-bed ion exchanger to insure that the treated water meets the required quality criteria. The 6.81 m<sup>3</sup>/min (1800 gpm) deionization plant has the capability of producing deionized water of 2 000,000 ohms/cm.

Demineralized water is distributed, as needed, to the hydrogen generation plant and the VHTR nuclear heat source. An 3030 m<sup>3</sup> (800,000 gal) stainless steel storage tank provides surge capacity for the demineralized water make-up.

Wastes from the water make-up systems must be treated prior to discharge. These wastes include spent regenerant solutions from the demineralization system, backwash effluent from the filters, and clarifier bottoms.

The waste regenerant solutions will discharge to one of two tanks where it will be neutralized to a pH value of approximately 7 by the addition of an alkali or acid as required. The neutralized solution can then be discharged.

Backwash effluent from the filters will be recycled through the clarifier.

The clarifier bottoms discharge will consist of a precipitated sludge containing about 3 percent solids by weight. This stream will be conveyed to a "thickener" where the solids will be further concentrated to about 25-30 percent. The concentrated stream is filtered using a rotary drum type vacuum filter. The resulting sludge - about 18,000 kg/day (20 tons/day) - contains about 50 percent solids by weight and is conveyed by truck to ultimate off-site disposal.

#### 4.5.2.10 Electrical Auxiliary Power System

The electrical auxiliary power system provides the facilities to distribute power to the electrolyzers and process equipment in the plant. Normal power sources are the gas and steam turbines in the plant complex as well as the small power recovery turbines in the SO<sub>2</sub>/O<sub>2</sub> separation system. Emergency and/or start-up power is supplied by an external 138 kV connection to the electric utility system.

During normal operation, the plant is electrically self-sufficient. All electric power needed for operation of the VHTR and hydrogen production facilities is generated on-site, with no excess power for sale nor need to import power.

#### 4.5.2.11 General Facilities

Included in the category of general facilities are things like site improvements, miscellaneous buildings (e.g., administration, control, maintenance and service, warehouse, etc.) certain auxiliary systems (e.g., instrument and plant air, fire protection, space heating boiler, sanitary sewage system, communications equipment, etc.) and certain facilities or equipment (e.g., furniture, fixtures, maintenance tools and equipment, laboratory equipment, etc.).

The general facilities, where applicable and appropriate, are shared between the VHTR nuclear heat source and the hydrogen production plant.

#### 4.5.3 Plant Performance Characteristics

The performance of the plant can be expressed in several ways. The paragraphs below summarize the performance in terms of resource consumption, process outflows, and overall thermal efficiency. The performance, relative to other hydrogen generation processes, is summarized in Section 5.

##### 4.5.3.1 Resource Consumption

For purposes of evaluation, the only resources considered are those associated with the operation of the plant, and not with the manufacture or construction of the facility. The resources are categorized into fuel ( $U_3O_8$ , thorium, and graphite for the VHTR), consumptive water use, and chemicals and catalysts. Table 4.5.9 summarizes the annual consumption of these materials. Since all electrical power is generated on-site, no electrical "resource", i.e., off-site facility is charged to the evaluation. It is assumed that all catalysts will be replaced annually. The major make-up chemical is sulfur which is assumed to require make-up at the rate of two system inventories per year.

TABLE 4.5.9  
NUCLEAR WATER DECOMPOSITION  
ANNUAL RESOURCE CONSUMPTION  
(80% Capacity Factor)

Water	$1.95 \times 10^{10}$ kg	$(4.3 \times 10^{10})$ lb)
Catalysts and Chemicals	$4.35 \times 10^5$ kg	$(9.6 \times 10^5)$ lb)
Uranium Ore ( $U_3O_8$ )	$1.81 \times 10^5$ kg	$(4.0 \times 10^5)$ lb)
Thorium (fertile material)	$8.50 \times 10^3$ kg	$(1.9 \times 10^6)$ lb)
Graphite (VHTR moderator)	$9.10 \times 10^4$ kg	$(2.0 \times 10^5)$ lb)

#### 4.5.3.2 Process Outflows

The major process product stream, in addition to hydrogen, is oxygen. This gas is produced at the rate of 305,000 kg/hr (673,500 lb/hr) and, for the purpose of the evaluation, is assumed to be vented.

#### 4.5.3.3 Process Thermal Efficiency

Thermal efficiency, as presented in Table 4.5.10, is defined as the higher heating value of the product gas divided by the heat input to the total plant complex. Since the plant is self-sufficient from an energy viewpoint, i.e., no net sale or purchase of power or heat is required for operation of the VHTR and hydrogen plant, the heat input is the full thermal rating of the VHTR. As in the other hydrogen generation processes, the work of compression of the product gas to 6895 kPa (1000 psia) is included in the calculation of efficiency.

The efficiency calculated is that which results from the process flowsheet and parameters selected for this phase of the evaluation. As discussed in Section 4.6, the efficiency will change as basic operating parameters are altered, e.g., process temperature, pressure, etc.

TABLE 4.5.10  
NUCLEAR WATER DECOMPOSITION  
OVERALL PROCESS EFFICIENCY

<u>Heat Input</u>		
VHTR Thermal Output	11,592 GJ/hr	(10.99 x 10 <sup>9</sup> Btu/hr)
<u>Heat Output</u>		
Product Gas	4.23 x 10 <sup>5</sup> std m <sup>3</sup> /hr	(15.8 x 10 <sup>6</sup> SCF/hr)
Heating Value	12.79 MJ/std m <sup>3</sup>	(325 Btu/SCF)
Total Heat Output	5410 GJ/hr	(5.135 x 10 <sup>9</sup> Btu/hr)
<u>Overall Efficiency</u>		
	$\frac{5410 \text{ GJ/hr} \times 100}{11,592 \text{ GJ/hr}}$	46.7%



#### 4.5.4 Process Performance Sensitivity Analysis

Sensitivity studies were conducted using the University of Kentucky HYDRGN computer program suitably modified to simulate the major features of the Westinghouse Hydrogen Generation Process. An optimum set of process conditions was determined by maximizing the thermal efficiency over a range of process variables. A schematic of the process flowsheet used in the sensitivity study is shown in Figure 4.5.4, with the major process steps identified in Table 4.5.11.

Hydrogen is provided electrolytically according to the following reaction:



The sulfuric acid formed is sent to a surge tank, ST, from which it is fed to two vaporizers, one recuperatively heated - AV-1, and the other externally heated - AV-2.

The resultant sulfur trioxide - steam mixture is sent to the thermal reduction reactor, where sulfur dioxide and oxygen are formed. This gas mixture ( $\text{SO}_3$ ,  $\text{SO}_2$ ,  $\text{O}_2$ ,  $\text{H}_2\text{O}$ ) is subsequently cooled and the unreacted sulfur trioxide is condensed as sulfuric acid. The sulfuric acid is recovered and recycled to the surge tank. The remaining wet sulfur dioxide and oxygen flow to the separation system. Steam is first condensed and recycled. The sulfur dioxide - oxygen mixture is compressed to 5171 kPa (750 psia) and separated with the recovery of sulfur dioxide for recycle to the electrolyzer. Oxygen is available as a by-product.

For each of the above steps there is an associated enthalpy change - dependent upon such process conditions as pressure, temperature, and acid concentration - which influences the overall thermal requirements of the process. The determination of those process conditions which lead to the lowest total heat input requires an analysis of each step of the process.

Several important tradeoffs exist in specifying process conditions. One relates to the concentration of the sulfuric acid leaving the electrolyzer. The electrolyzer power requirement increases with increasing acid concentration, as shown in Figure 4.5.5. As Figure 4.5.6 indicates, the energy required to heat, vaporize, and decompose the electrolyzer acid (Steps 4, 5, 6 and 7 in Figure 4.5.4) diminishes with increasing acid concentration. Figure 4.5.7 shows that mass rates also decline with an increase in acid concentration. Analogously, operation at very low acid concentrations lowers the electrolyzer power requirements, but leads to high mass rates and thermal demands in the acid decomposition loop. An optimal acid concentration exists.

This optimum acid concentration can be expected to be a function of the temperature of heat source driving the process. The electrolyzer power, for example, can be generated more efficiently with thermal energy at higher temperatures. Similarly, higher temperatures enable higher conversions per pass to be obtained in the  $\text{SO}_3$  decomposition reactor, thereby reducing the recycle rates in this part of the system.

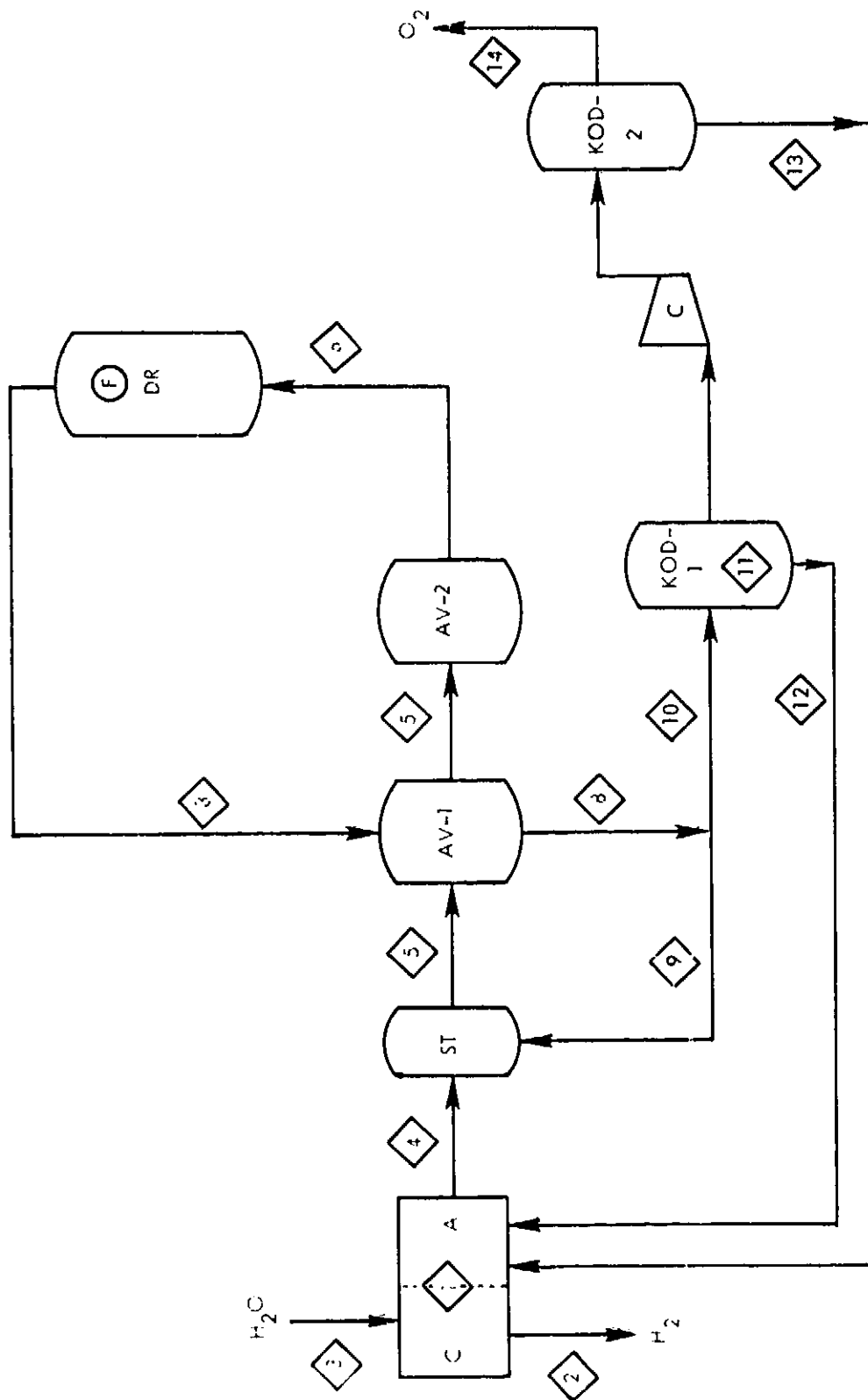


Figure 4.5.4 Flowsheet for H<sub>2</sub> Generation Process  
(Based on Sensitivity Study Simulation)

TABLE 4.5.11  
PROCESS STEPS

- 1 Electrolysis:  

$$2\text{H}_2\text{O} + \text{SO}_2 \longrightarrow \text{H}_2 + \text{H}_2\text{SO}_4$$
- 2 Cooling of  $\text{H}_2$  from electrolyzer temperature (360K) to 298 K, collection of  $\text{H}_2$
- 3 Heating make-up water to 360K for electrolyzer
- 4 Heating dilute sulfuric acid (from electrolyzer) from 360K to its boiling point
- 5 Vaporization of the dilute  $\text{H}_2\text{SO}_4$
- 6 Heating  $\text{H}_2\text{SO}_4(\text{g})$  and  $\text{H}_2\text{O}(\text{g})$  to the temperature of decomposition reactor
- 7 Decomposing  $\text{H}_2\text{SO}_4$  into  $\text{H}_2\text{O}$  and  $\text{SO}_3$ , then decomposing  $\text{SO}_3$  to  $\text{SO}_2$  and  $1/2 \text{O}_2$
- 8 Cooling gas mixture from DR to the temperature at which unreacted  $\text{SO}_3$  condenses as dilute  $\text{H}_2\text{SO}_4$
- 9 Condensation of unreacted  $\text{SO}_3$  as dilute acid; recycling this acid to the surge tank
- 10 Cooling  $\text{H}_2\text{O}$ ,  $\text{SO}_2$ ,  $\text{O}_2$  gas mixture to the temperature at which  $\text{H}_2\text{O}$  condenses
- 11 Condensation of  $\text{H}_2\text{O}$ ; Separation of  $\text{SO}_2 - \text{O}_2$  mixture
- 12 Cooling water to 360 K for recycle to electrolyzer
- 13 Cooling  $\text{SO}_2$  to 360 K for recycle to electrolyzer
- 14 Cooling  $\text{O}_2$  to 298 K for venting

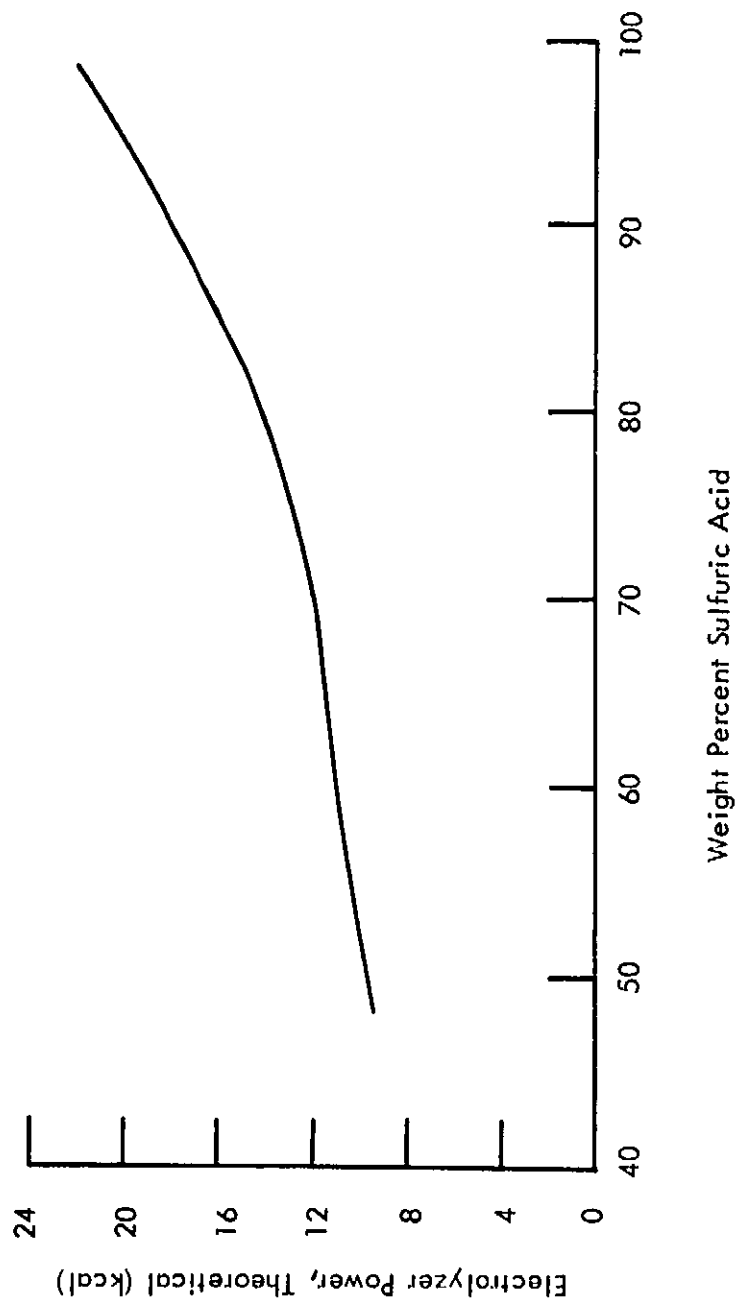


Figure 4.5.5 Variation in Theoretical Electrolyzer Power with Acid Concentration

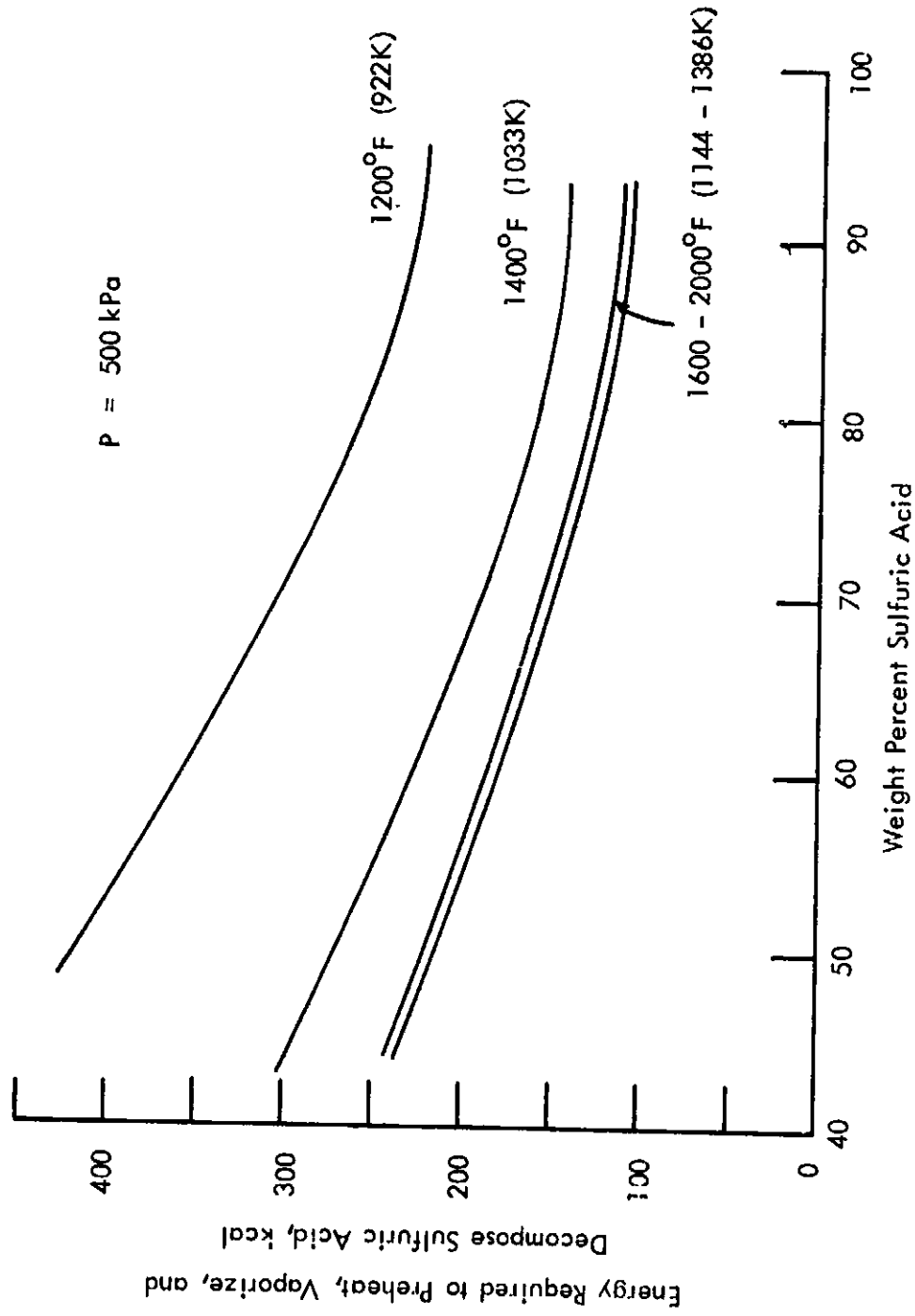


Figure 4.5.6 Variation in Acid Decomposition Energy with Acid Concentration

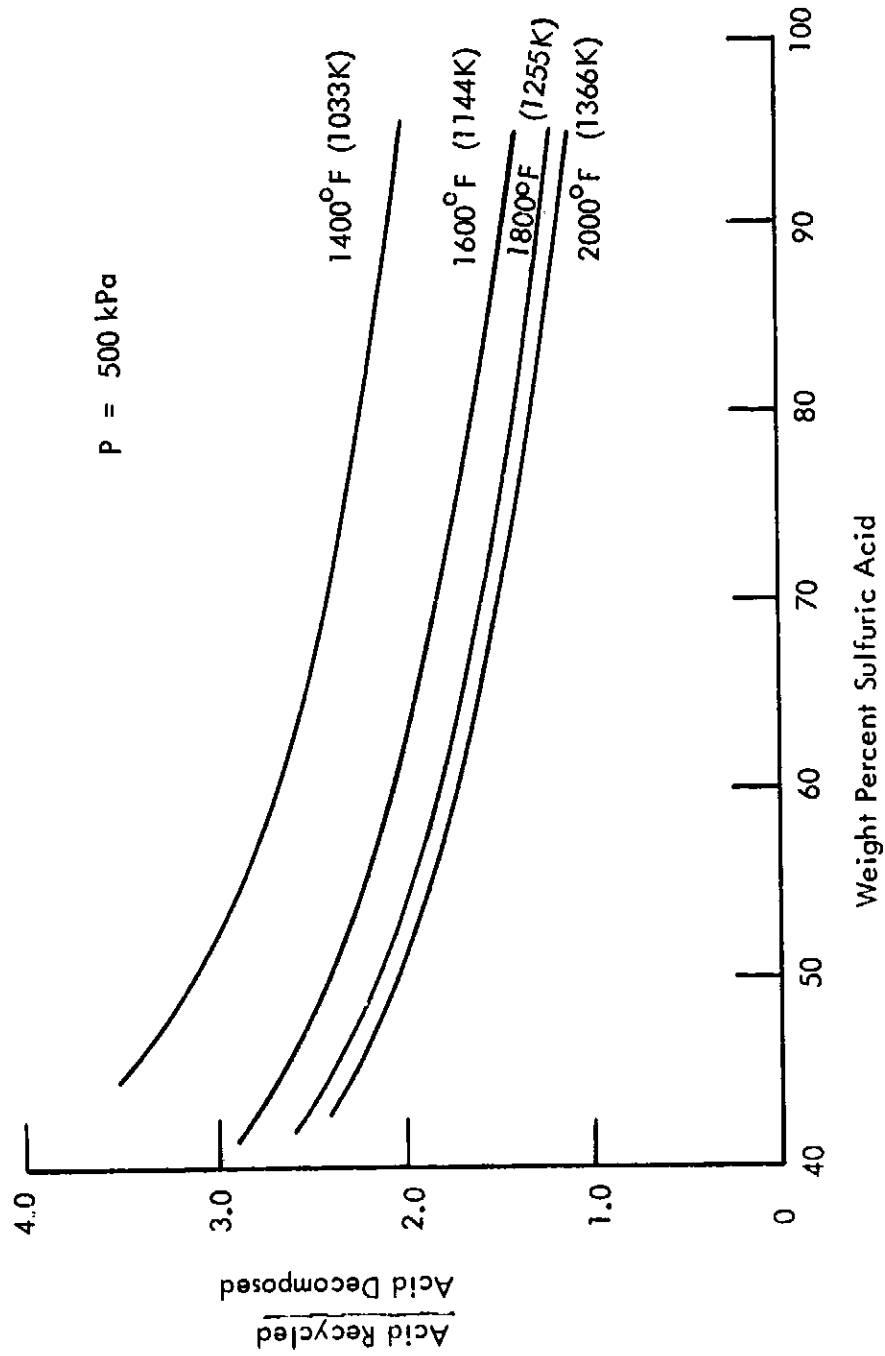


Figure 4.5.7 Variation of Recycle Rate with Acid Concentration

Pressure is important due to the pressurized sulfur dioxide - oxygen recovery system employed in the process as well as the pressure dependence of the sulfur trioxide reduction reactors (the equilibrium conversion at a given temperature declines with increasing system pressure). As Figure 4.5.8 shows, recycle rates increase with increasing pressure. Similarly, operation at low pressures leads to high conversions, low recycle rates, and large compression requirements. Thus, an optimal pressure also exists.

The optimum pressure is also a function of temperature. For a given conversion per pass, an increase in temperature permits the use of a higher decomposition system pressure. Referring to Figure 4.5.9, where details of the compression system are shown, this reduces the number of compression stages required in the  $\text{SO}_2 - \text{O}_2$  separation system. As Figure 4.5.9 shows, operation of the decomposition system at pressures above 1010 kPa (10 atm) can achieve significant reductions in compression energy.

The preceding section indicates trends in thermal requirements produced by varying the process conditions over selected ranges. Knowledge of the total heat requirement,  $Q_T$ , is necessary to determine process efficiency. The smaller  $Q_T$ , the higher the efficiency.  $Q_T$  is a function of process conditions and can be reduced by using recuperative heat exchange, whereby heat released in exothermic steps is used to supply those steps requiring heat. The major recuperative heat exchange occurs in AV-1 (see Figure 4.5.4) where the energy in streams 8 and 9 is used to preheat the vaporize acid entering the  $\text{SO}_3$  decomposition system.

Estimates of the process thermal efficiency were made for a range of process conditions. These were generated by choosing five values for each of three critical process variables, pressure, temperature, and acid concentration, as shown in Table 4.5.12. Based on these variables, 125 processes were generated, each one uniquely determined by its combination of values for the process conditions.

TABLE 4.5.12  
VARIATIONS IN PROCESS CONDITIONS

Pressure (kPa)	DR Temperature (K)	Acid Concentration (wt percent)
101	922	50
507	1033	60
1013	1144	70
2026	1255	80
5065	1366	90

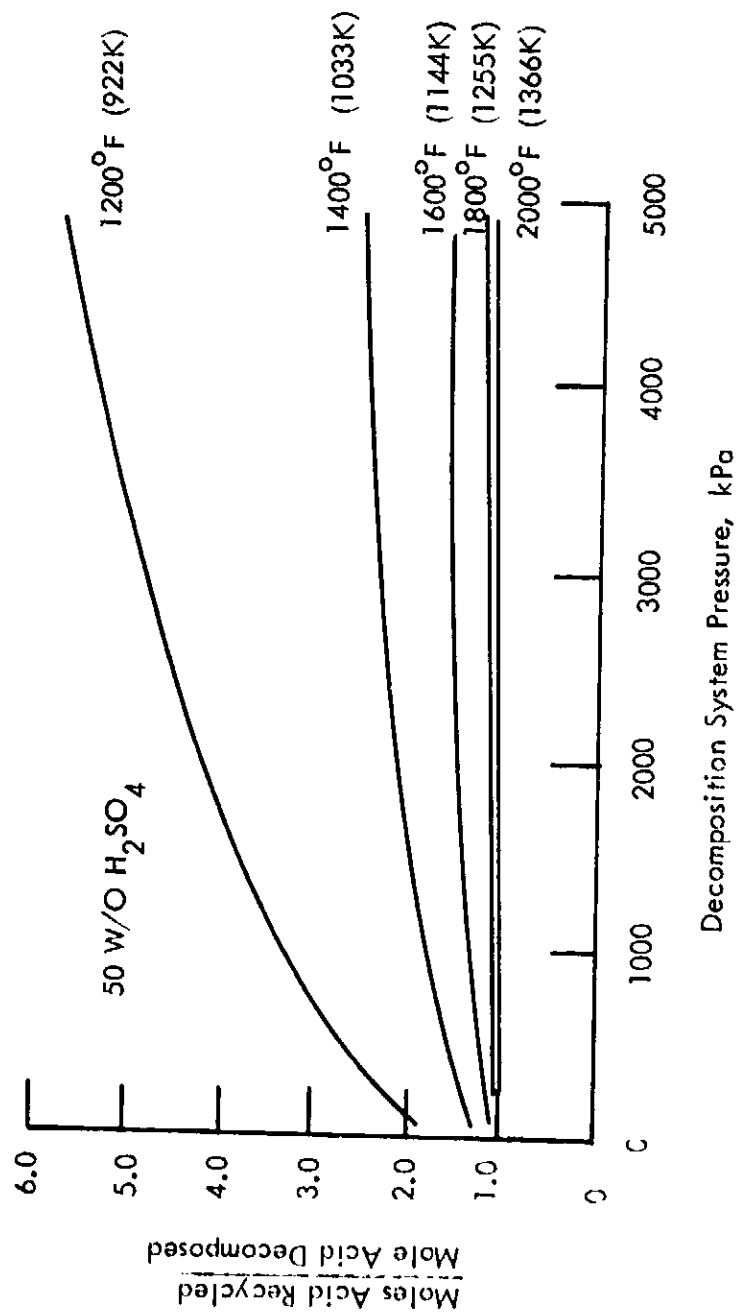


Figure 4.5.8 Variation of Recycle Rate with Pressure



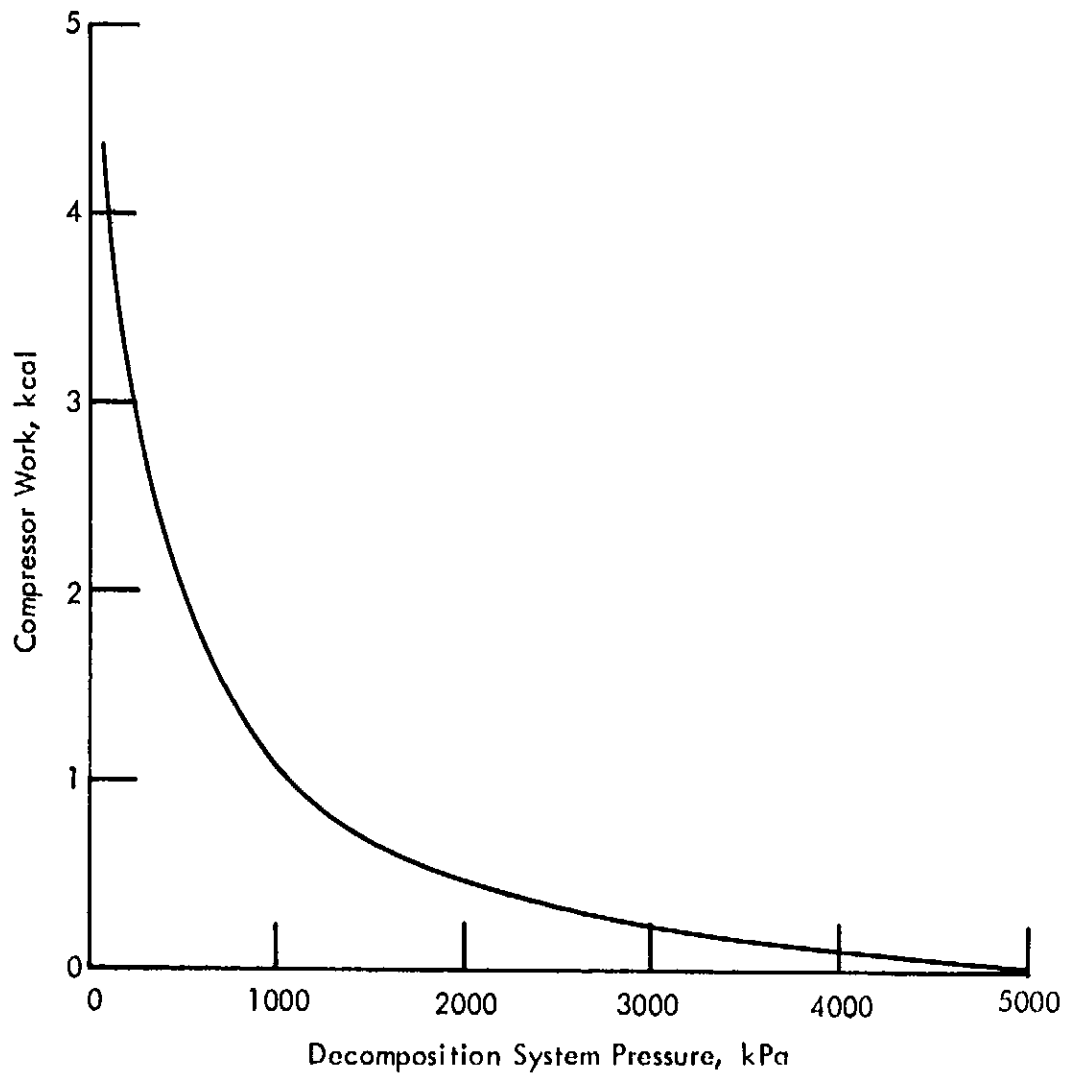


Figure 4.5.9 Variation of  $\text{SO}_2/\text{O}_2$  Separation System Compressor Requirements with Decomposition System Pressure

The total energy required by each of these processes was considered to be composed of three parts. The first of these, designated  $Q_1$ , represents the heat required to generate the electrolyzer power. Both an electrolyzer efficiency and a power generation efficiency were assumed in calculating  $Q_1$ . Specifically, the electrolyzer efficiency was assumed to be 50 percent. The power generation efficiencies were typical of those achievable using a combined gas and steam turbine cycle operating at a temperature 139K (250°F) above that of the process temperature. The second heat input,  $Q_2$ , represents the net heat required to heat, vaporize, and decompose the electrolyzer acid (4 + 5 + 6 + 7 - 8 - 9). The third input is  $Q_3$ , the heat requirement for the  $SO_2 - O_2$  separation process, which was calculated as described above in Figure 4.5.9.

Figures 4.5.10 and 4.5.11 are plots of efficiency as a function of pressure and acid concentration, respectively. The optimum combination of conditions, as determined within the limits of this study, is the following: pressure between 1013 and 2026 kPa (10 and 20 atm) and acid concentration between 70 and 85 w/o.

Not unexpectedly, the analysis shows (Figure 4.5.12) overall thermal efficiency to increase monotonically with temperature. Similarly (Figure 4.5.13), the thermal energy exchanged in the recuperative vaporizer (a measure of the recycle rate in the acid decomposition loop) decreases hyperbolically with temperature. At low temperatures, 922 to 1033K (1200 - 1400°F), system pressure strongly influences the size of the recycle system. At high temperatures, 1255 to 1266K (1800 - 2000°F), pressure is important, with the lower range, 103 to 517 kPa (15 to 75 psia), being preferred.

The process thermal efficiency also varies with electrolyzer efficiency and the type of power generation equipment employed (Figure 4.5.14).

Operation of the electrolyzers at higher efficiencies, corresponding to lower current densities and more expensive capital equipment, raises overall thermal efficiency and lowers the power generation requirements. Off-setting the more expensive electrolyzers is the lower capital cost made possible by the inclusion of additional gas turbine generating capacity, and lower operating costs achieved by improved thermal efficiency. This trade-off between electrolyzer efficiency and cost will be examined in more detail during the conceptual design study.

Throughout, it should be noted that the sensitivity analysis predicts lower thermal efficiencies than those obtained by analysis of the engineering flowsheets. This may be understood by referring to Figure 4.5.4. In the sensitivity study, no heat is assumed to be recovered from Step 10. In actuality, Step 10 is used for steam generation to supply the sulfur dioxide vaporizer and the compressor turbine driver steam requirements. Similarly, after separation of  $SO_2$ , an oxygen stream at nominally 4877 to 5171 kPa (700 to 750 psia) is available. Power recovery is affected in expanding this gas to 101 kPa (one atmosphere) prior to venting. In the sensitivity analysis, these effects are neglected as they are features common to all process variations, and as such do not alter conclusions concerning the relative effects of changing process parameters.

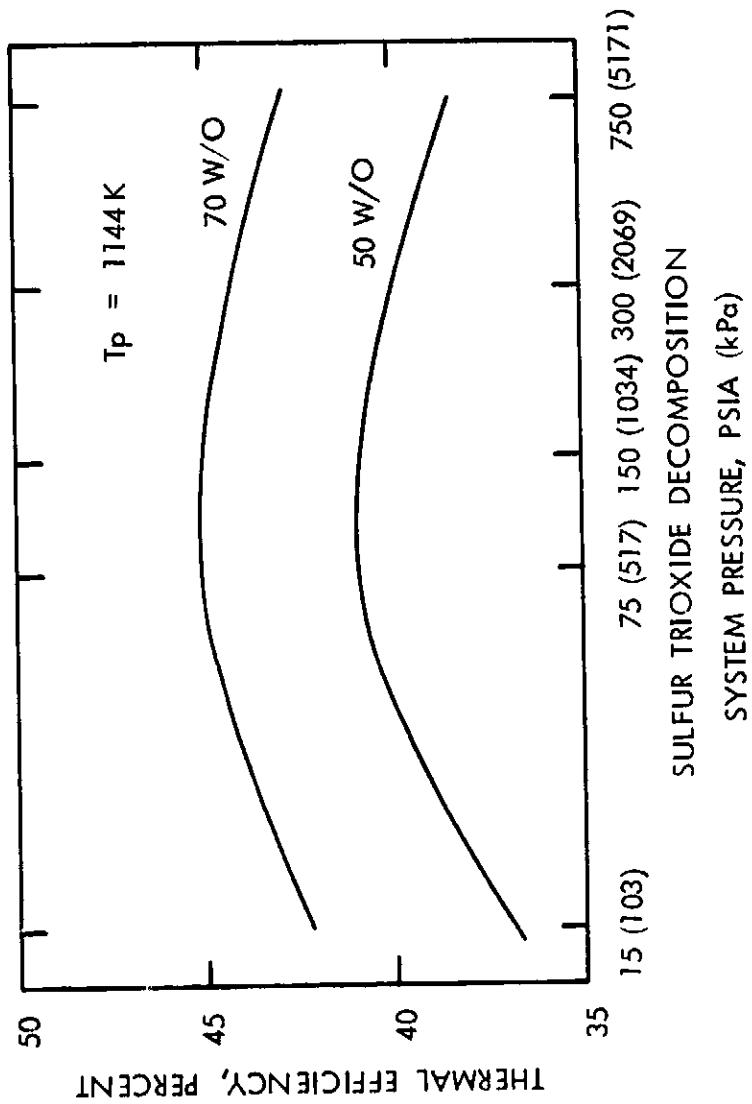


Figure 4.5.10 Variation of Process Thermal Efficiency with Pressure

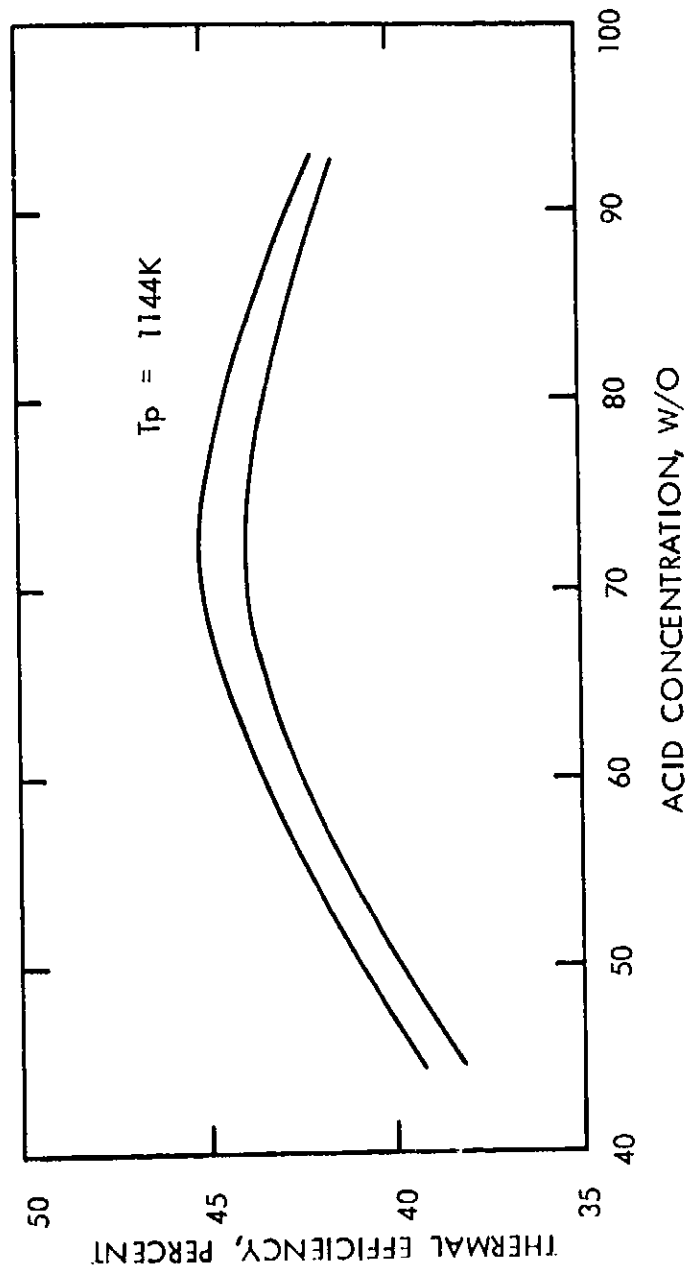


Figure 4.5.11 Variation of Process Thermal Efficiency with Acid Concentration

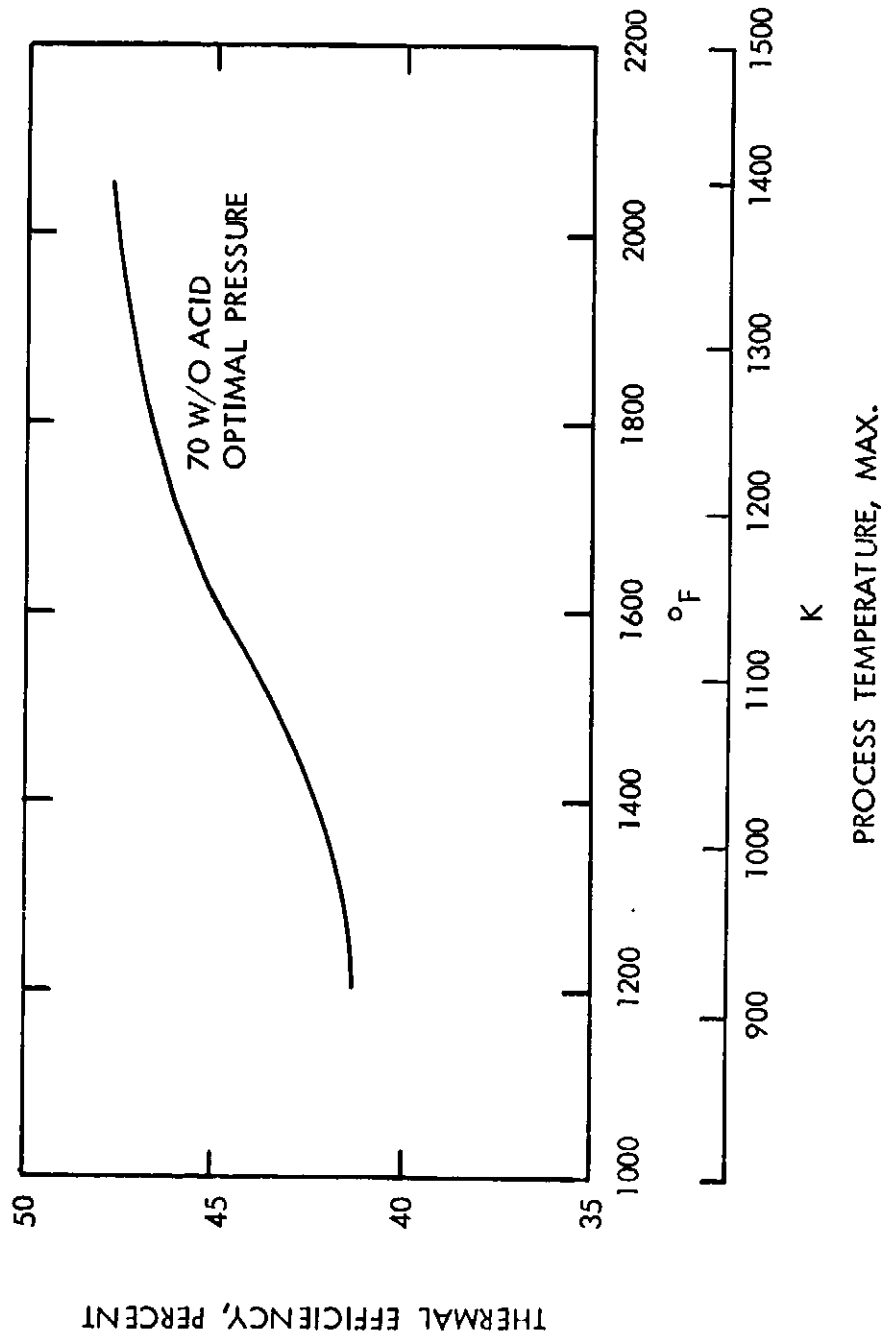


Figure 4.5.12 Variation of Process Thermal Efficiency with Process Gas Temperature

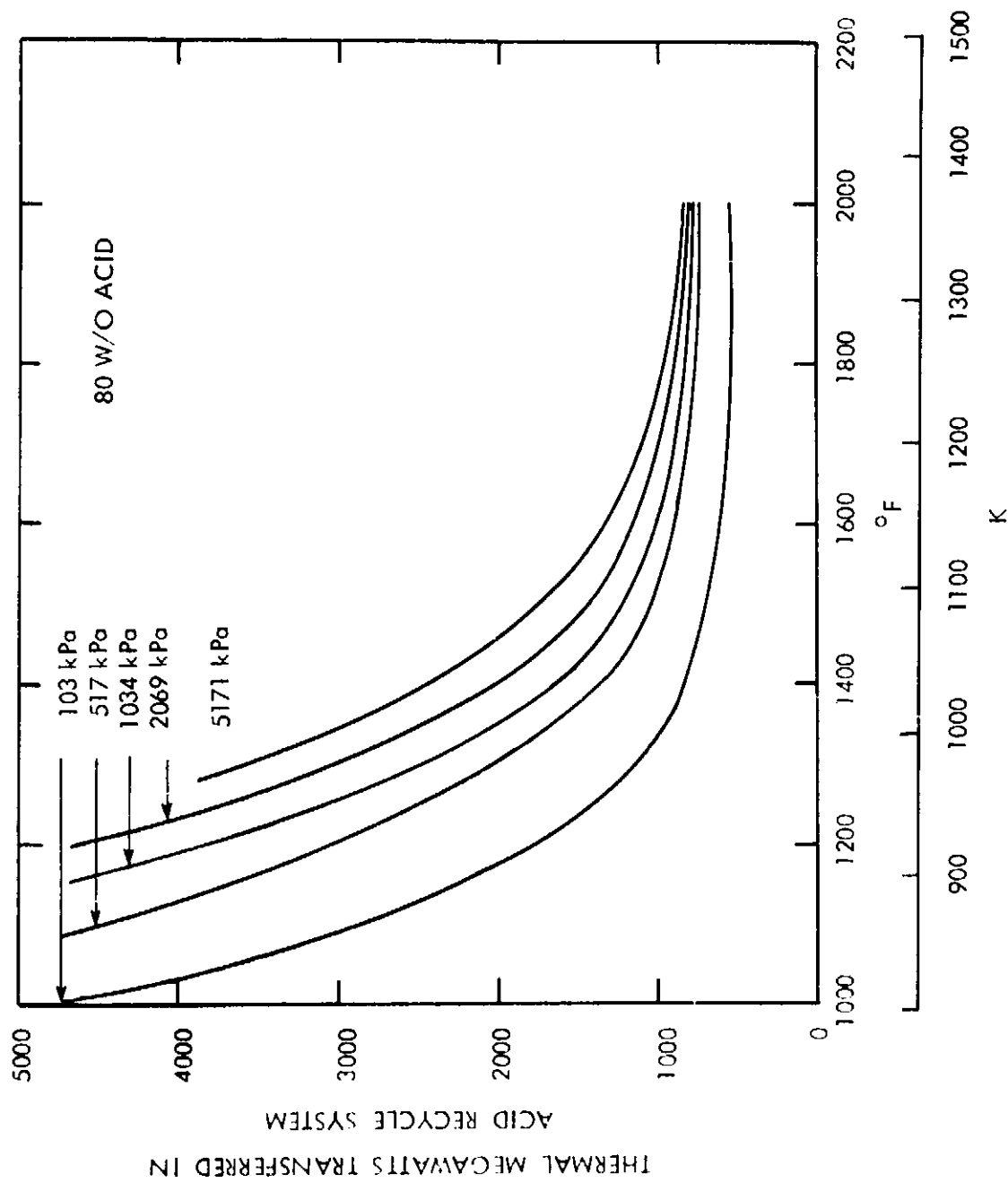


Figure 4.5.13 Energy Recycle as a Function of Process Temperature

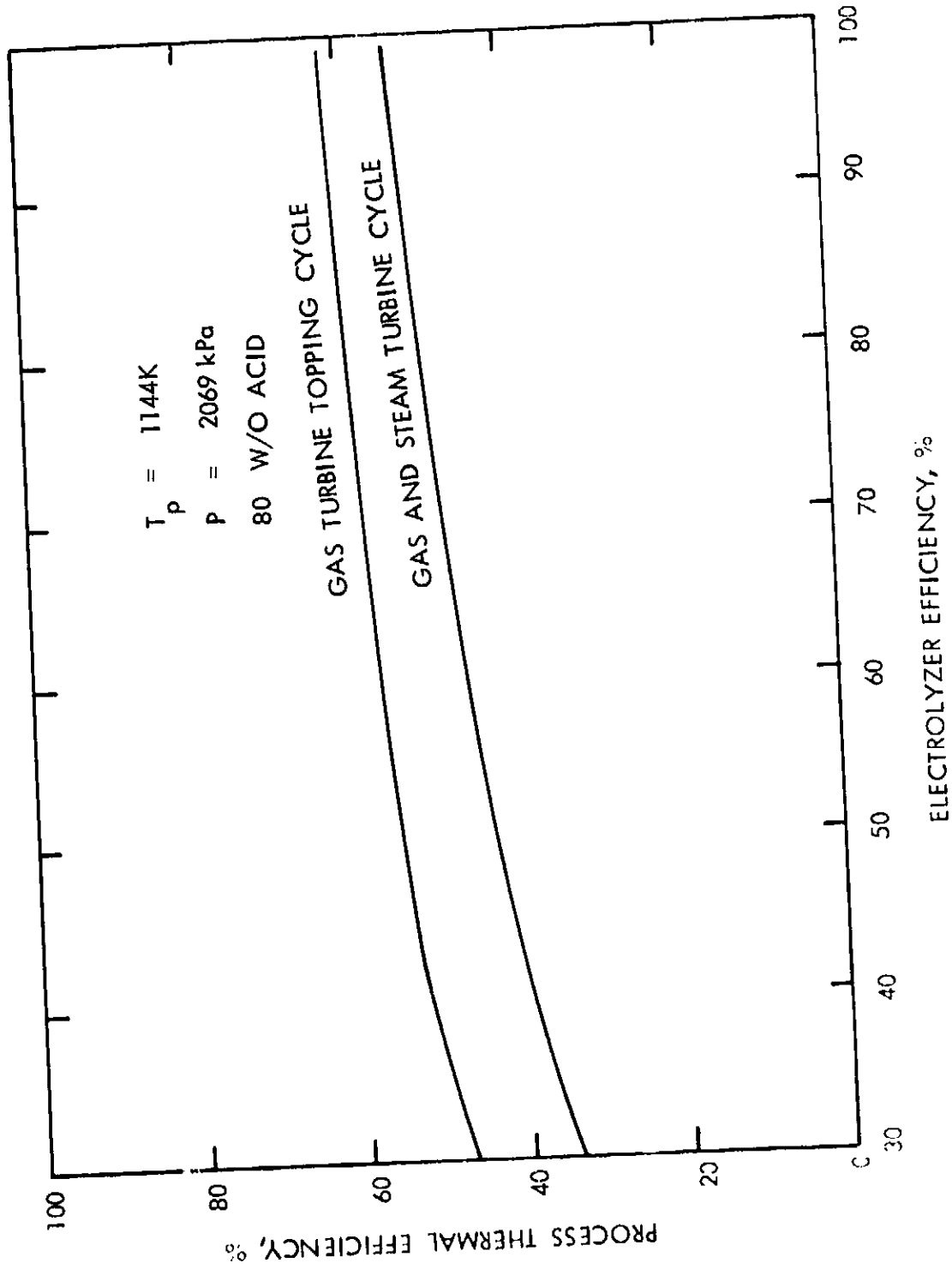


Figure 4.5.14 Variation of Process Thermal Efficiency with Electrolyzer Efficiency

The true value of thermal efficiency is affected, however, by these factors. This effect amounts to about a five percent decrease in the absolute magnitude of the process thermal efficiency as calculated by the computer process simulation. Thus a value of 42 percent computed during the sensitivity analysis translates to about 47 percent when actual flowsheets are prepared.

#### 4.5.5 Economics

The cost of producing hydrogen is evaluated for the plant design discussed in Sections 4.5.1 and 4.5.2. In determining the overall costs, estimates were made of the capital, operation and maintenance, and fuel costs for the facility in the general format used in reporting nuclear powerplant costs, as defined in NUS-531 (Reference 32). The costs of the VHTR nuclear heat source were taken from the ERDA sponsored conceptual design study reported in Reference 1. These costs were adjusted to account for the interfacing of the VHTR with the hydrogen production plant. The effects on the production costs of different capacity factors, fuel costs, and type of ownership were also considered.

##### 4.5.5.1 Capital Costs

The capital costs estimate is based on preliminary sizing of most of the major plant equipment and determining appropriate costs for that equipment. Factors, based on experience with these types of systems, were used to account for the costs of installation, piping, valves, instrumentation, structures, and miscellaneous equipment. Indirect costs were also estimated by applying factors in the manner described below.

The VHTR costs used in the economic evaluation were taken from Reference 1 and adjusted to account for refinements in the interface conditions, inclusion of the intermediate coolant loop piping and circulators, and upgrading of the reactor rating from 3000 to 3220 Mw(t). The VHTR direct costs, as reported in Reference 1 as used in this evaluation, are shown in Table 4.5.13.

The hydrogen production plant, producing  $10.15 \times 10^6$  standard  $m^3$ /day ( $379 \times 10^6$  SCFD), is estimated to require a direct cost investment, in mid-1974 dollars, of \$315,418,000, as shown in Table 4.5.14. The direct cost is presented according to a code of accounts that divides systems among on-sites and off sites, with the former relating to closely related mainline processing steps and the latter consisting of support and service systems and facilities. The off-sites accounts reflect the consideration that the VHTR and hydrogen plant are at the same location, resulting in shared services, buildings, and facilities. The off-sites, therefore, consist of the incremental costs, relative to that already included in the VHTR costs to provide the required services.

The total plant investment, shown in Table 4.5.15, includes the direct costs plus contingencies, indirect costs, and interest during construction. For the purpose of evaluation, land and land rights are shown separately from other direct costs since it is a non-depreciating asset.



TABLE 4.5.13  
 NUCLEAR HEAT SOURCE (VHTR)  
 DIRECT CAPITAL COSTS  
 (July 1974 Dollars)

Account <sup>(1)</sup>	Item	Installed Cost (\$ Thousand) <sup>(2)</sup>		Remarks
		Reference	This Study	
20	Land and Land Rights	\$ 800	\$ 800	
21	Structures and Site Facilities			
211	Site Improvements and Facilities	2,515	2,515	
212	Reactor Building	16,196	16,600	Increased Plant Rating
214	Intake and Discharge Structures	798	-	Cooling Tower Instead of River Cooling
215	Reactor Auxiliary Building	25,009	25,500	Increased Plant Rating
216	Control and Electrical Building	4,065	4,065	
217	Diesel Generator Building	1,932	1,932	
218	Administration Service Building	851	851	
219	Helium Storage Building	180	275	Storage for Helium in Intermediate Loop
22	Reactor Plant Equipment			
221	Reactor Equipment	63,401	65,670	Increased Rating
222	Main Heat Transfer and Transport System	73,844	90,500	Increased Rating. Inclusion of Intermediate Loop Equipment
223	Safeguards Cooling Systems	4,965	5,700	Increased Rating
224	Radioactive Waste Treatment	2,332	2,400	Increased Rating
225	Nuclear Fuel Handling and Storage	13,213	13,300	Increased Rating
226	Other Reactor Plant Equipment	12,057	12,400	Increased Rating, Intermediate Loop Helium Purification
227	Instrumentation and Control	8,796	8,900	Intermediate Loop Control
24	Electric Plant Equipment			
241	Switchgear	1,373	1,447	Intermediate Loop
242	Station Service Equipment	3,477	3,656	Intermediate Loop
243	Switchboards	695	710	Intermediate Loop
244	Protective Equipment	303	303	
245	Electrical Structures and Wiring Containers	3,309	3,410	Intermediate Loop
246	Power and Control Wiring	8,285	8,620	Intermediate Loop
25	Miscellaneous Plant Equipment			
251	Transportation and Lifting Equipment	1,278	1,278	
252	Air and Water Service Systems	5,131	6,455	Cooling Tower Instead of River Cooling
253	Communications Equipment	171	171	
254	Furnishings and Fixtures	145	145	
	Total Direct Cost	\$255,322	\$272,244	

(1) Account Numbers are those for Nuclear Plants as Determined by NRC Regulatory Guide 1.40.

(2) Includes Contingency Within Each Account.

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TABLE 4.5.14  
 WATER DECOMPOSITION PLANT  
 DIRECT CAPITAL COSTS  
 (July 1974 Dollars)

<u>Account</u>	<u>Item</u>	<u>Installed Cost ( \$ Thousands )</u>
<u>2000</u>	<u>On-Sites</u>	
2100	Battery F - Electrolyzer Power Supply	\$ 18,452
2200	Battery G - Electrolyzers	112,659
2300	Battery H - Sulfuric Acid Decomposition	82,814
2400	Battery I - SO <sub>2</sub> /O <sub>2</sub> Separation	28,670
2500	Battery J - Turbine-Generator	30,610
2600	Battery K - Hydrogen Product Compressors	<u>5,076</u>
	On-Sites Subtotal	\$ 278,281
<u>1000</u>	<u>Off-Sites</u>	
1100	Cooling System and Water Intake	\$ 6,204
1200	Make-Up and Feedwater	6,862
1300	Waste Water Treatment	301
1400	Coal Handling	N/A
1500	Steam Generation	See Battery J
1600	Electrical Auxiliary Power	17,484
1700	General Off-Sites Investment <sup>(1)</sup>	
1710	Land and Land Rights	200
1720	Site Improvements and Facilities	954
1730	Administration/Service/Laboratory Buildings	1,269
1740	Instrument and Plant Air	2,350
1750	Maintenance Facilities	432
1760	Fire Protection, Communications	846
1770	Furnishings, Fixtures, Laboratory Equipment	<u>235</u>
	Off-Sites Subtotal	\$ 37,137
	Total Direct Capital Cost	\$ 315,418

(1) Cost are incremental to comparable accounts in the VHTR estimate.

TABLE 4.5.15  
 NUCLEAR WATER DECOMPOSITION  
 ESTIMATED CAPITAL COST SUMMARY  
 (In Thousands of Dollars)

<u>Non-Depreciating Assets</u>	<u>VHTR</u>	<u>Water Decomposition</u>
Land and Land Rights	\$ 800	\$ 200
<u>Depreciating Assets</u>		
Special Materials	300	383
Physical Plant	<u>276,444</u>	<u>315,218</u>
Subtotal	\$ 276,744	\$ 315,601
Contingency	(Included Above)	<u>47,340</u>
Subtotal	\$ 276,744	\$ 362,941
<u>Indirect Costs</u>		
Construction Facilities, Equipment and Services	\$ 17,660	\$ 9,073
Engineering Services	\$ 43,376	\$ 14,518
Other Costs	\$ 13,435	\$ 3,629
Interest During Construction	<u>\$ 95,479</u>	<u>\$ 63,085</u>
Subtotal	\$ 169,950	\$ 90,305
Total Depreciating Asset	\$ 446,694	\$ 453,246
Total Plant Investment	\$ 900,940	

Special materials comprise the initial supply of chemicals, catalysts, lubricants and other materials needed for operation of the plant. A contingency of 15 percent is applied, for the hydrogen generation facilities, to the estimated cost of the special materials and the direct cost of the physical plant. Contingencies are included within the VHTR direct cost estimate.

Indirect costs are expense items of a general nature which apply to the overall project of building an operable plant, rather than to one of the direct costs. These costs, except for interest during construction, have not been estimated in detail, but calculated as a percentage of the direct costs based on the procedure defined in NUS-531 and updated by ERDA in 1974 for use in the study reported in Reference 1. The indirect costs for the water decomposition facilities are calculated as incremental costs to that already included in the VHTR estimate.

Construction facilities, equipment, and services include general costs associated with the plant construction, such as field offices, warehouses, temporary power and utility lines, cost or rental of construction equipment and supplies, purchase of electric power, water, and other utilities, security guards, training programs for the labor force, inspection and testing of construction materials, site cleanup, insurance, and the like.

Engineering services include items such as preliminary investigations; site selection; air and water environmental studies; subsurface investigations; preparation of specifications and evaluation of proposals for major equipment packages, preparation of preliminary and final design documents, design reviews, procurement, inspection, and expediting of materials and equipment; preparation of pre-operational test and plant startup procedures; assistance in securing plant permits; management and direction of construction activities, including selection of subcontractors, scheduling, maintaining cost and quality control; on-site procurement and receiving of materials and equipment; field accounting; supervising and pre-operational testing of systems and components; field engineering inspection of construction work to assure compliance with plans and specifications; and preparation of as-built drawings.

Other costs include the owner's property and all-risk insurance, state and local property taxes on the site and improvements during construction, sales taxes on purchased materials and equipment, staff training, plant startup, and the owner's general and administrative (G&A) costs.

Interest during construction is calculated as simple interest, at an 8 percent annual rate, on the plant investment as it is made. For the purpose of the evaluation, it is assumed that the land is purchased six months prior to the start of the project and that special materials are delivered and paid for nine months prior to plant commercial operation. The remainder of the plant investment is made as design and construction proceeds. Figure 4.5.15 shows the rate of expenditures as a fraction of time. The overall project period of eight years is

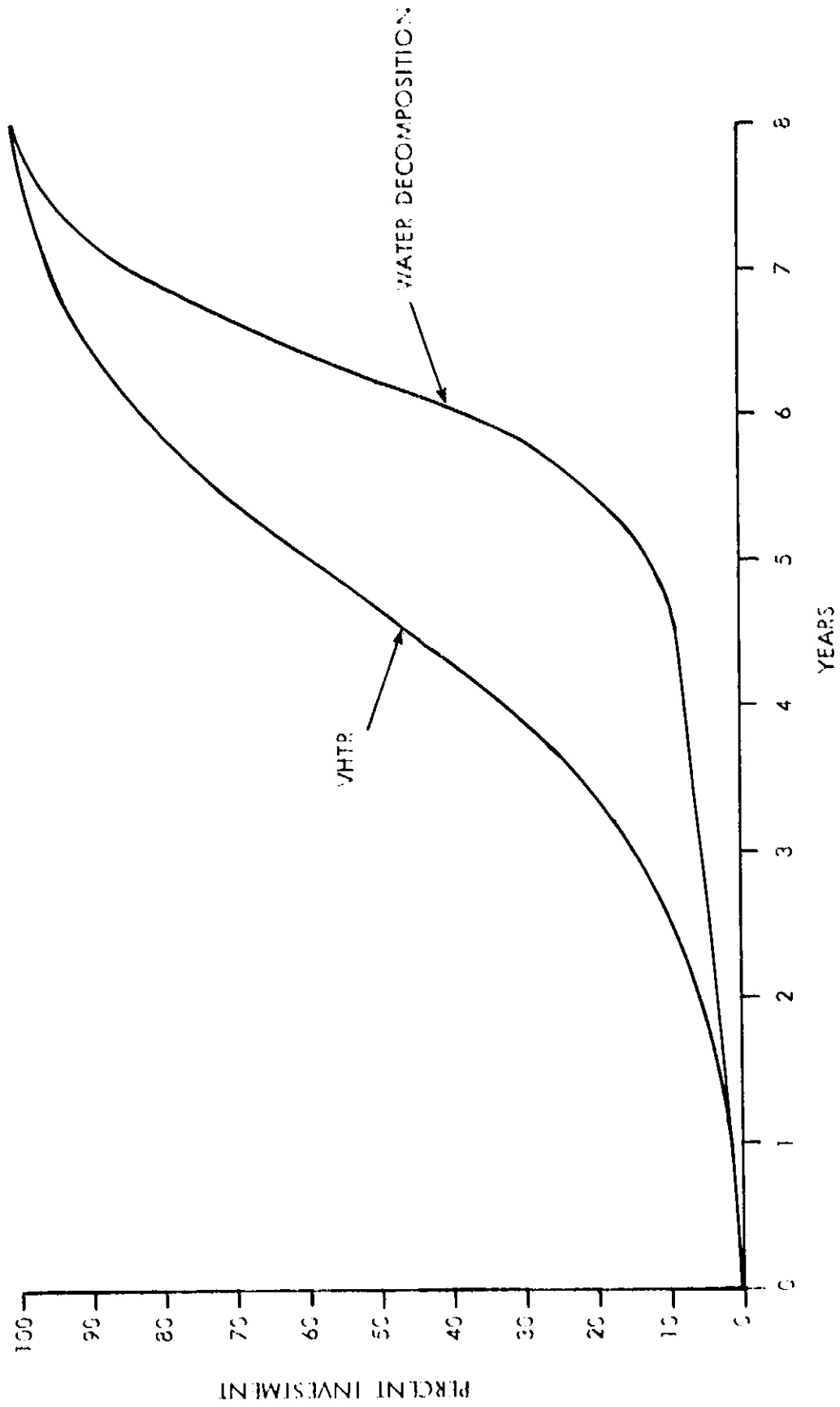


Figure 4.5.15 Nuclear Water Decomposition - Plant Capital Investment Expenditures Versus Time

dictated by the design, licensing, and construction time for the VHTR. The water decomposition plant requires a shorter construction time, and therefore the major investments in that part of the facility are delayed so that a common completion of construction can be achieved. Engineering and the development of information required for environmental impact statements and construction permits for the water decomposition plant proceeds in parallel with the comparable effort for the VHTR to assure that no schedular delays occur.

The total plant investment, including all direct and indirect costs but excluding escalation, is estimated to be \$900,940,000 for the grass roots facility.

#### 4.5.5.2 Operation and Maintenance Costs

The costs of operation and maintenance includes the expense of maintaining a plant staff, consumable supplies and equipment, outside support services, miscellaneous items of cost, and indirect costs of maintaining the plant working capital.

The direct O&M costs are shown in Table 4.5.16, as the costs estimated for the VHTR (Reference 1), plus the incremental costs for the water decomposition plant. The staff costs are based on a 140 person staffing level for the combined VHTR and water decomposition plant at an average cost of \$19,300 per man-year. The costs of chemicals and catalysts are based on their assumed use rate. An allowance has been included for miscellaneous consumables.

Outside support services are taken to embrace all services obtained other than from the normal plant complement during normal working hours. This includes personnel from other locations, as well as the cost of station personnel working overtime on special tasks such as refueling and equipment maintenance or repair. Other requirements for outside support services include such items as film-badge processing, laundering of contaminated clothing, off-site disposal of wastes, major equipment overhauls, and consultants to provide various forms of operational support. An allowance equal to 50 percent of the VHTR costs is used for these costs attributed to the water decomposition plant.

Miscellaneous O&M costs include such items as:

- training new staff personnel,
- requalification of operators,
- rent (for property, equipment, or facilities which are used or occupied in connection with plant operation),
- travel, such as to staff conferences at the main office, or to professional society meetings or other conferences,

TABLE 4.5.16

NUCLEAR WATER DECOMPOSITION  
DIRECT ANNUAL O & M COSTS

<u>Staff Payroll</u>		\$ 2,702,000
VHTR	\$ 1,544,000	
H <sub>2</sub> Plant	\$ 1,158,000	
<u>Consumable Supplies and Equipment</u>		\$ 928,000
VHTR	\$ 435,000	
H <sub>2</sub> Plant	\$ 493,000	
<u>Outside Support Services</u>		\$ 210,000
VHTR	\$ 140,000	
H <sub>2</sub> Plant	\$ 70,000	
<u>Miscellaneous</u>		\$ 120,000
VHTR	\$ 80,000	
H <sub>2</sub> Plant	\$ 40,000	
	Subtotal	\$ 3,960,000
<u>G &amp; A</u>		\$ 594,000
<u>Nuclear Liability Insurance</u>		\$ 390,000
	Total Direct O & M Costs	\$ 4,944,000

- licenses and fees,
- office-supplies, postage, and telephone/telegraph bills, and
- fuel and upkeep of station vehicles.

As before, an allowance of 50 percent of the VHTR costs is used for the water decomposition plant.

An annual premium of \$390,000 is assumed for nuclear liability insurance. This premium is in addition to other insurance premiums included in the annual charge on capital, as shown in Section 4.1.2.

The total direct annual operation and maintenance cost of \$4,944,000 includes a 15 percent G&A assessment on all costs, except for nuclear liability insurance.

The indirect O&M costs are shown in Table 4.5.17. These are the costs of maintaining the working capital required for continued operation of the plant and is evaluated at a 10 percent annual charge rate. The working capital is made up of the cash in hand needed to meet the day to day operating expenses plus the value of materials and supplies in inventory. The average net cash required is calculated at 2.7 percent of the direct O&M costs, less the nuclear insurance premium. A two month supply of consumables is assumed to be kept in inventory. To account for pre-payment of nuclear insurance, 50 percent of the premium is included as working capital.

The total O&M costs, at a plant capacity factor of 80 percent, are shown in Table 4.5.18.

#### 4.5.5.3 Fuel Costs

Fuel costs are all expenses associated with the nuclear fuel cycle of the VHTR. These include items such as procurement of all materials, uranium enrichment, fuel fabrication, fuel reprocessing, credits for materials of value in spent fuel, and carrying charges in all parts of the fuel cycle. The fuel cycle costs, as reported in Reference 1, in accordance with the economic groundrules of Section 4.1.2, is 24.75¢/GJ (26.1¢/10<sup>6</sup> Btu).

The plant, operating at an 80 percent capacity factor and a thermal output of 3220 mw, will accumulate a total annual fuel cost of \$20,071,000.

#### 4.5.5.4 Hydrogen Production Costs

The hydrogen production cost is made up of the contributions of capital, operation and maintenance, and fuel costs. These are normally calculated on an annual basis. The percentage of the plant investment that is charged against production each year is a function



TABLE 4.5.17  
 NUCLEAR WATER DECOMPOSITION  
 INDIRECT OPERATION AND MAINTENANCE COSTS

	<u>Cost</u>
Average Net Cash Required	\$ 123,000
Materials and Supplies In Inventory	
Consumable Supplies and Equipment	\$ 155,000
50% of Nuclear Liability Insurance Premium	195,000
Total Working Capital	\$ 473,000
Annual Charge Rate	10%
Annual Indirect O & M Cost	\$ 47,300

TABLE 4.5.18  
 NUCLEAR WATER DECOMPOSITION  
 TOTAL ANNUAL O & M COST  
 (80% Capacity Factor)

	<u>Cost</u>
Direct O & M Costs	\$ 4,944,000
Indirect O & M Costs	<u>47,300</u>
Total	\$ 4,991,300

TABLE 4.5.19

## NUCLEAR WATER DECOMPOSITION

## HYDROGEN PRODUCTION COST COMPARISON

(80% Capacity Factor)

<u>Annual Costs</u>	<u>Ownership</u>	
	<u>Utility</u>	<u>Industrial</u>
Non-Depreciating Capital	\$ 100,000	\$ 100,000
Depreciating Capital	134,991,000	224,985,000
Operation and Maintenance	4,991,300	4,991,300
"Fuel"	<u>20,071,000</u>	<u>20,071,000</u>
Total Annual Cost	\$ 160,153,000	\$ 250,147,300
 <u>Annual Gas Production</u>	 2.96 x 10 <sup>9</sup> std m <sup>3</sup> (1.107 x 10 <sup>11</sup> SCF)	 2.96 x 10 <sup>9</sup> std m <sup>3</sup> (1.107 x 10 <sup>11</sup> SCF)
 <u>Production Cost</u>	 5.4¢/std m <sup>3</sup> (\$1.45/MSCF) \$4.22/GJ (\$4.45/10 <sup>6</sup> Btu)	 8.5¢/std m <sup>3</sup> (\$2.26 MSCF) \$6.59 GJ (\$6.95/10 <sup>6</sup> Btu)

of the type of plant ownership, i.e., utility or industrial, and the manner in which the owner can do business. As discussed in Section 4.1.2, the annual charge on non-depreciating assets, e.g., land, is 10 percent for either type of ownership while the annual charge on depreciating assets is 15 percent for utility ownership and 25 percent for industrial ownership. Although production costs are calculated on both a utility and industrial basis, it is not realistic to consider that the production of hydrogen, on the scale contemplated and with distribution to remote "users", would be an "industrial" enterprise. It is considered that this sort of production plant would much more readily fit a "regulated utility" type of enterprise - much like today's natural gas and electric utility operations.

The cost of hydrogen production, on both bases, is shown in Table 4.5.19. As can be seen, the cost, which is equivalent to a "gate selling price", is 5.4¢ standard m<sup>3</sup> (\$1.45/MSCF), or \$4.22/GJ (\$4.45/10<sup>6</sup> Btu) on a utility basis. The cost to the ultimate consumer would be this production cost plus the allocated capital and operating costs of transmission and distribution.

#### 4.5.5.5 Sensitivity of Hydrogen Production Costs to Variables

The cost of hydrogen production from any given plant will vary with the cost of fuel, the type of ownership, and the utilization, i.e., capacity factor, of the facility. For the base case calculation, it was assumed that fuel costs were 24.75¢/GJ (26.1¢/10<sup>6</sup> Btu), the capacity factor was 80 percent, and utility ownership prevailed.

Figure 4.5.16 shows the effect on hydrogen production cost of variations in the cost of fuel for both utility and industrial ownership, with the capacity factor remaining at 80 percent as in the base case. The effect the production cost of hydrogen, if the oxygen was sold instead of vented, is shown for one assumed value of the oxygen.

Table 4.5.20 indicates the manner in which the capacity factor affects the production cost. In this table, all of the cost assumptions are the same as the base case with only the capacity factor allowed to vary within a range of 40 to 90 percent. As can be seen, the cost of capital remains constant regardless of how the plant is operated. Operation and maintenance costs are divided into two parts, i.e., fixed and variable. The fixed costs are independent of the plant performance and accrue whether or not the plant is operated. The variable costs are a direct function of the plant operation. Nuclear fuel costs also have fixed and variable components.

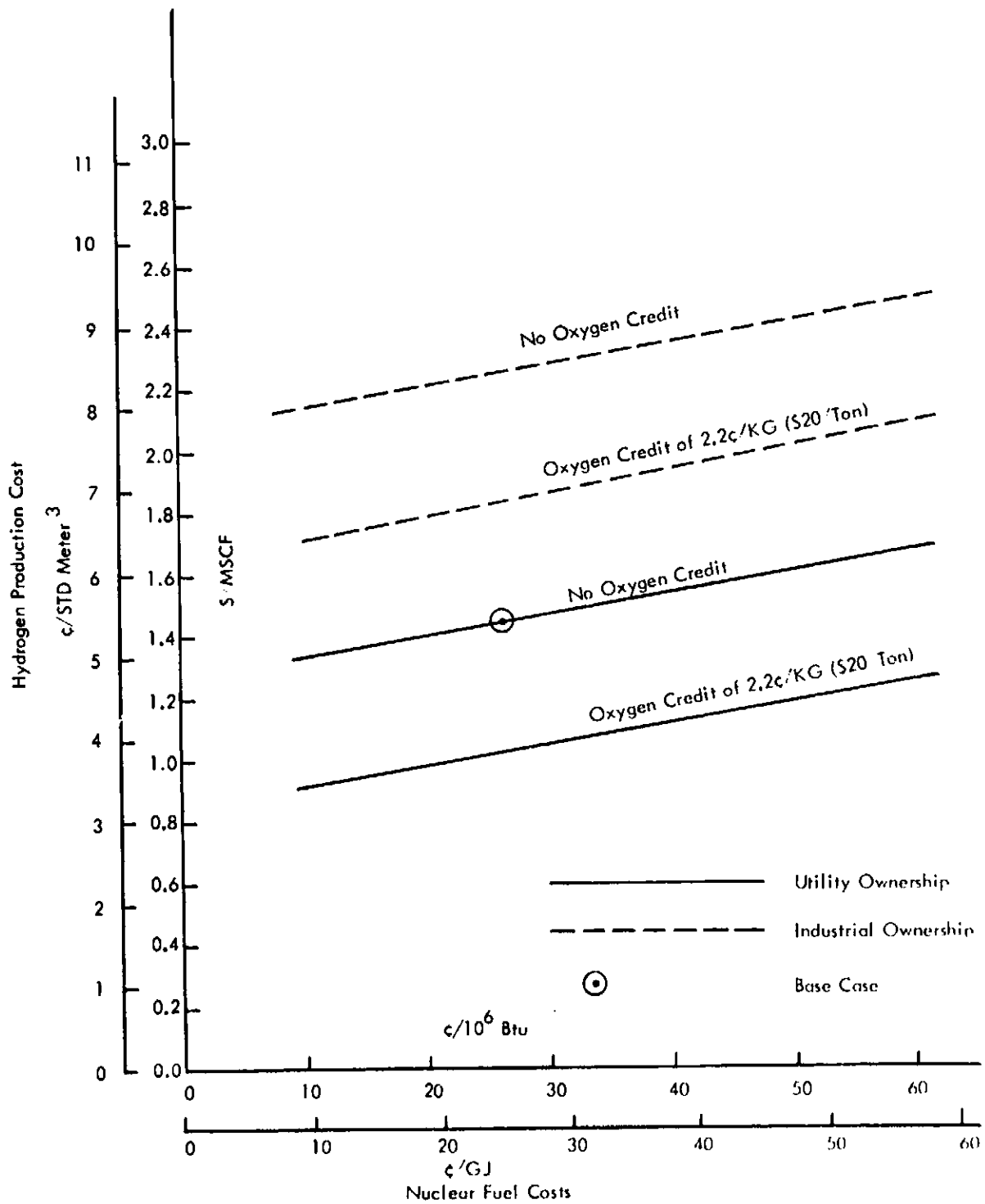


Figure 4.5.16 Nuclear Water Decomposition Hydrogen Cost Versus Nuclear Fuel Cost (80% Capacity Factor)

TABLE 4.5.20  
 NUCLEAR WATER DECOMPOSITION  
 SENSITIVITY OF H<sub>2</sub> PRODUCTION COST TO CAPACITY FACTOR  
 (Base Case Cost Assumptions)

Item	Capacity Factor		
	40%	60%	80%
Capital Cost	\$ 135,091,000	\$ 135,091,000	\$ 135,091,000
Fixed O & M	3,975,000	3,975,000	3,975,000
Variable O & M	558,000	837,000	1,016,000
Fixed Fuel Costs	6,363,000	6,363,000	6,363,000
Variable Fuel Costs	6,854,000	10,281,000	13,708,000
Total Annual Cost	\$ 152,841,000	\$ 156,547,000	\$ 162,107,000
Annual Gas Production	1.48 x 10 <sup>9</sup> std m <sup>3</sup>	2.22 x 10 <sup>9</sup> std m <sup>3</sup>	2.96 x 10 <sup>9</sup> std m <sup>3</sup>
	(5.54 x 10 <sup>10</sup> SCF)	(8.30 x 10 <sup>10</sup> SCF)	(1.107 x 10 <sup>11</sup> SCF)
Production Cost	10.33¢/std m <sup>3</sup>	7.05¢/std m <sup>3</sup>	4.87¢/std m <sup>3</sup>
	(\$2.76/MSCF)	(\$1.89/MSCF)	(\$1.45/MSCF)
			3.33 x 10 <sup>9</sup> std m <sup>3</sup>
			(1.245 x 10 <sup>11</sup> SCF)

## 5.0 COMPARATIVE EVALUATION OF HYDROGEN PRODUCTION PROCESSES

### 5.1 GENERAL

The hydrogen production systems selected for evaluation were water electrolysis, coal gasification using Koppers-Totzek and Bi-Gas gasifiers, and a nuclear driven water decomposition system. Each of these systems has its own unique operating characteristics, advantages, and disadvantages that make a definitive comparison between systems, to determine the "overall best", indeed difficult. Some of the systems are commercially available today - others require many years of development to achieve technical viability. The systems yet to be demonstrated hold the greatest promise for efficient utilization of natural resources and economic attractiveness.

Since the weighing of individual performance, environmental, and economic factors is subjective, no attempt has been made to rank the system from "best" to "worst." Rather, the factors important to a comparative evaluation are presented for interpretation by any reader. The factors include the technical readiness and development requirements, economics, and resource utilization and environmental impact potential.

Although no conclusions are drawn relative to the "best" hydrogen generation system, it is obvious that the potential value of the nuclear water decomposition system, in terms of economics, resource conservation, environmental impact potential, and overall effectiveness warrants continued and expanded definition of the process and development of the key process steps. Accordingly, the effort under Task III of this contract, to be reported separately, will consist of a more detailed conceptual design of the nuclear water decomposition system and a definition of the development program, in terms of tasks, schedules, and cost, required for full scale demonstration of the process.

### 5.2 COMPARISON OF TECHNOLOGICAL READINESS AND DEVELOPMENT REQUIREMENTS

With regard to technological readiness, two distinct categories can be defined:

1. Water electrolysis and Koppers-Totzek coal gasification are "here today" technologies with demonstrated technical viability for hydrogen production.
2. Nuclear water decomposition and Bi-Gas coal gasification are promising technologies for hydrogen production; both need development work to bring them to the technological maturity enjoyed at present by electrolysis and K-T gasification.

#### 5.2.1 Water Electrolysis

Water electrolysis has a broad based technical background with commercial units on the market today. Where the cost of electricity is relatively low and local

uses of hydrogen exist, electrolysis is used to provide on-site hydrogen generation. Commercial units cover a size range from portable units (<1 liter/min) to tons of hydrogen per day. Recent development work has been stimulated by related fuel cell technologies which use the reverse electrochemical reaction. The state-of-the-art of electrolysis has been advanced by the fuel cell work via development of electrodes with low polarization, by low internal resistance cell design and by reductions in size and weight of components. Applications of some of the above items to conventional water electrolysis systems have resulted in changes in operating parameters, reduced power consumptions, and/or reduced capital costs. Improvements in operating efficiency may be achieved by use of noble metal catalyzed electrodes or by the use of higher operating temperatures. So far the high costs of catalyzed electrodes offset any advantage gained, but the search for new low cost catalysts is continuing. For the present, further efficiency improvements will come from the development and application of low cost, easily fabricated materials that will allow higher operating temperatures to be used.

With this development background in mind, it should be recalled that water electrolysis has fundamental thermodynamic limits in its performance potential. One limit is dictated by the ideal electrochemical reaction energy,  $\sim 68$  kcal/mole. The other limit is dictated by the overall thermal efficiency of the power plant. Thus, further technological advances in water electrolysis will be bounded by these constraining limits.

### 5.2.2 Koppers-Totzek Coal Gasification

Koppers-Totzek gasification is a commercially available process which is adaptable for the production of synthesis gas for hydrogen, ammonia, methanol, methane, or gasoline production, low-Btu fuel gas, or substitute natural gas.

The Koppers-Totzek process uses the entrained concurrent flow principle based on the partial combustion of pulverized coal in oxygen and steam. In 1948, Koppers-Essen and Koppers-Pittsburgh, in a joint effort, used this concept in the design of a one ton per hour pilot plant gasifier. The pilot plant was built for the U.S. Bureau of Mines, and the first successful run of the gasifier was made more than 25 years ago. The pilot plant was operated over a period of two years to yield liquid hydrocarbon from the Koppers-Totzek synthesis gas. The first commercial Koppers-Totzek gasifier was installed in Finland in 1952 and was followed by plants in various parts of the world.

The heart of the K-T process is the gasifier. Koppers Company offers both a two-headed gasifier capable of handling 15000 kg/hr (400 tpd) of coal and a four-headed gasifier capable of handling 32000 kg/hr (850 tpd). In the two-headed gasifier, burner heads are 180 degrees apart; in the four-headed gasifier, they are 90 degrees apart. The gasifier, shaped like spheroidal cones centrally welded together, has a double-walled shell constructed of boiler quality plate. A set of burners is mounted at the apex of each gasifier cone.

The synthesis gas from the gasifier, after cleaning and cooling, is processed in the manner consistent with the desired end product. For the generation of a hydrogen product, the processing steps include sulfur and acid gas removal, carbon monoxide shift, carbon dioxide removal, and methanation.

Several features of the K-T process make it particularly attractive for hydrogen generation from coal. Because it is a commercially successful system, the technology of the process, including materials requirements, operating procedures, and performance characteristics are both well known and predictable. In addition, the downstream processing steps use commercially available technologies, catalysts, and predictable performance and economics. The process also has considerable flexibility in the choice of fuel to be gasified.

The disadvantages of the K-T process involve limits in the capacity and operating pressure of the gasifiers resulting in a multiplicity of units for large plants and affecting the capital and operating costs of the facility.

There are privately funded programs underway to overcome these disadvantages. Larger gasifiers are being developed. A small pressurized entrained gasifier, designed for up to 3040 kPa (30 atm) operation, has been tested and has indicated that commercial operation at pressure is feasible.

### 5.2.3 Bi-Gas Coal Gasification

The Bi-Gas process is being developed primarily for production of high Btu pipeline quality gas with ~95% methane in the final product stream. If used primarily for hydrogen production, the Bi-Gas process must undergo some modification from its original purpose.

Development work on Bi-Gas by Bituminous Coal Research, Inc., has proceeded from batch-type experiments through continuous flow experiments in a 5-pound per hour external heated reactor, to operation of a process and equipment development unit (PEDU). Research has confirmed the basic assumption that high yields of methane could be obtained from coal at elevated temperatures and pressures.

With the completion of the PEDU test program, plans were made to design a larger-scale, fully integrated 5-ton per hour gasification pilot plant at Homer City, Pennsylvania. Bids for the detailed engineering and construction of the pilot plant were received and the construction contract was awarded in 1972. Completion of construction of the pilot plant is scheduled for 1975. The overall objective of the pilot plant is to provide sufficient design data for construction of a commercial plant.

The heart of the Bi-Gas process is the two-stage gasifier. Pulverized coal is introduced into the upper section (Stage 2) at 70 to 100 atmospheres. Here the coal comes in contact with a rising stream of hot synthesis gas that has been produced in the lower



section (Stage 1). In Stage 2, the coal is partially converted to methane and more synthesis gas. The raw gas output from Stage 2 including entrained residual char is sent to waste heat boilers and char cyclone where the char is separated from the gas and recycled to Stage 1 of the gasifier. A portion of the synthesis gas is also recycled to both stages of the gasifier.

The pilot plant will serve to verify the performance of the two stage gasifier. Testing with the plant's gasifier should demonstrate that a high pressure, 1200K (1700°F) synthesis gas can indeed be produced and that design and calculational models used heretofore for the gasifier are adequate. Several other aspects of the process are in the development stage and will be evaluated during testing of the pilot plant. These areas include coal feeding, slag removal, char separation, CO shifting, acid gas removal and methanation. Most of the above process items are germane if the process were to be tailored to produce hydrogen. In addition, as a hydrogen producing plant, additional development of the process would be required to verify feasibility. Included would be the steps of cryogenic separation of the methane and hydrogen, with subsequent expansion of the methane to lower pressure, steam/methane reforming, repressurization of the reforming product steam and feedback of this stream into the CO shift converter.

#### 5.2.4 Water Decomposition System

The technology of the water decomposition system is the least developed of the systems being considered for hydrogen production. Work performed to date, and the information generated from that work, continues to support the fundamental attractiveness of this hydrogen generation process. Using common, inexpensive chemicals, the cycle is capable of decomposing water at high efficiencies under a broad range of operating conditions. A considerable amount of flexibility exists in the selection of process temperature and pressure without seriously jeopardizing system performance. More importantly, the cycle consists of chemical reactions-verified by laboratory testing - that proceed as written and at rates sufficient to insure compact and economical chemical reactors.

The paragraphs below discuss the status of technology and development requirements for the nuclear heat source and the water decomposition system.

##### 5.2.4.1 The VHTR Nuclear Heat Source

The very high temperature nuclear reactor (VHTR) is a graphite moderated, helium cooled unit drawing heavily upon the technology demonstrated in the AEC/NASA nuclear rocket program to provide the capability for the high temperatures needed for the water decomposition plant. The nuclear system also uses the technology developed and demonstrated in the HTGR and other gas cooled reactor programs to support its design concept. The conceptual design of the VHTR was supported by ERDA under Contract AT(11-1)-2445 and reported in Reference 1. The research and development program required to bring the VHTR to first large-scale demonstration was also defined

in Reference 1 and consisted of an 11.5 year program with total costs, in 1974 dollars, of \$240,600,000 excluding the cost of design of the demonstration plant.

#### 5.2.4.2 The Water Decomposition System

The technological status and development required of the water decomposition system can be categorized into two areas, i.e., materials and chemical process. The former represents an area within which all processes and developing technologies will live or die - the ability to define materials that will perform their function within the operating environment of the process. The latter represents the availability of information from which specific designs can be made that perform in accordance with predictions. A detailed R&D program recommendation will be prepared as part of the Task III effort under this contract.

##### 5.2.4.2.1 Materials Considerations

The materials investigation performed have been limited to the determination of unique or unusual materials requirements for the system described in Section 4.5. The critical problem areas involve the high temperature sulfuric acid loop shown in Figure 4.5.1. The remainder of the system operates at relatively low temperatures,  $<476\text{K}$  ( $<400^\circ\text{F}$ ) and thus can utilize commercially available components. The high temperature acid decomposition loop, because of the temperatures and pressures involved, departs significantly from standard sulfuric acid handling practice. Appendix A discusses the status of available materials.

##### 5.2.4.2.2 Technological Status of the Water Decomposition Hydrogen Generation Process

The efforts in examining the Westinghouse Sulfur Cycle water decomposition process have been devoted primarily to the two key process steps, i.e., the generation of hydrogen by the electrochemical reaction  $\text{SO}_2 + 2\text{H}_2\text{O} \longrightarrow \text{H}_2 + \text{H}_2\text{SO}_4$  and the generation of oxygen by the thermochemical reduction of sulfur trioxide in accordance with the reaction  $\text{SO}_3 \longrightarrow \text{SO}_2 + 1/2\text{O}_2$ . Work to date has been of a nature to confirm that the primary reactions do proceed, to determine the nature and degree of competing reactions to define and identify specific subsystems for further consideration and evaluation, and to provide a preliminary assessment of process feasibility.

Information gathered to date continues to support the fundamental attractiveness of this hydrogen generation process. Using common, inexpensive chemicals, the cycle is capable of decomposing water at high efficiencies under a broad range of operating conditions. More importantly, the cycle consists of chemical reactions - verified by laboratory testing - that proceed as written and at rates sufficient to insure compact and economical chemical reactors.

A discussion of pertinent experimental data related to the technology of the Sulfur Cycle water decomposition system appears in Appendix B.

### 5.3 ECONOMIC COMPARISON OF HYDROGEN PRODUCTION PROCESSES

The comparative economic evaluation attempts to treat all four hydrogen systems in a consistent manner in respect to the major items that constitute the cost of hydrogen production. These are capital, operation and maintenance, and energy costs. The sensitivity of the cost of hydrogen to plant ownership (utility or industrial), nuclear fuel and coal cost, purchased electric power cost, by-product credits, and capacity factor are also evaluated.

#### 5.3.1 Capital Costs

The capital costs for the four hydrogen production plants, derived in Section 4, are summarized in Table 5.3.1.

For water electrolysis, the capital cost reflects a projected price level for a package consisting of electrolyzers, associated equipment, and certain engineering services. With a large proportion of the direct cost supplied in this fashion, a ten percent contingency was used. Engineering services costs reflect the inclusion, in the direct cost, of appreciable systems engineering effort by the electrolyzer vendor. Interest during construction was based on an assumed overall four year project period with a non-linear rate of expenditure. The total cost indicated does not include the cost of a dedicated light water nuclear power station to provide power for the unit. This would add \$822,160,000 to the site investment.

The costs of Koppers Totzek and Bi-Gas coal gasification systems were estimated on a consistent basis. Both systems use downstream processing to produce hydrogen with only minor amounts of co-products. The Bi-Gas system, although not fully developed, holds promise of sufficiently higher gasifier output and reduced gasifier cost to more than compensate for the more extensive processing to produce high purity hydrogen. Interest during construction is based on an assumed overall six year project period with a non-linear rate of expenditure.

For nuclear water decomposition, the capital cost is shown for both the nuclear heat source (VHTR) and the water decomposition plant. The VHTR costs were taken from WANL-2445-1, "The Very High Temperature Reactor for Process Heat" (Reference 1) with adjustments to reflect:

- Increase in rating from 3000 MWt to 3220 MWt to preclude the need for purchased electric power.
- Inclusion of the equipment needed to interface with the water decomposition plant, e.g., intermediate loop piping and circulators.
- Other modifications, e.g., use of cooling tower instead of river cooling, make-up water supply transferred to water decomposition plant.

TABLE 5.3.1

COMPARISON OF CAPITAL COSTS (IN THOUSANDS OF DOLLARS)

	WATER ELECTROLYSIS		COAL GASIFICATION KOPPERS-TOTZEK BI-GAS		WATER DECOMPOSITION VHTR	
NON-DEPRECIATING ASSETS						
LAND AND LAND RIGHTS	\$ 800	\$ 1,000	\$ 1,000	\$ 1,000	\$ 800	\$ 200
DEPRECIATING ASSETS						
SPECIAL MATERIALS	\$ 1,933	\$ 2,992	\$ 2,992	\$ 3,285	\$ 300	\$ 383
PHYSICAL PLANT	\$ 351,462	\$ 259,676	\$ 229,308	\$ 229,308	\$ 276,444	\$ 315,218
		\$ 262,668	\$ 232,593	\$ 232,593	\$ 276,744	\$ 315,601
CONTINGENCY	\$ 53,009	\$ 39,400	\$ 34,889	\$ 34,889	(INCL. ABOVE)	\$ 47,340
		\$ 302,068	\$ 267,482	\$ 267,482	\$ 276,744	\$ 362,941
SUBTOTAL	\$ 406,404					
INDIRECT COSTS						
CONSTRUCTION FACILITIES, EQUIPMENT, AND SERVICES	\$ 22,356	\$ 17,022	\$ 15,247	\$ 15,247	\$ 17,660	\$ 9,073
ENGINEERING SERVICES	\$ 19,100	\$ 25,980	\$ 23,271	\$ 23,271	\$ 43,376	\$ 14,518
OTHER COSTS	\$ 13,414	\$ 8,541	\$ 7,649	\$ 7,649	\$ 13,435	\$ 3,629
INTEREST DURING CONSTRUCTION	\$ 43,319	\$ 52,684	\$ 45,861	\$ 45,861	\$ 95,479	\$ 63,085
INDIRECT COSTS	\$ 98,189	\$ 104,227	\$ 92,028	\$ 92,028	\$ 169,950	\$ 90,305
TOTAL DEPRECIATING ASSETS	\$ 504,593	\$ 406,295	\$ 359,510	\$ 359,510	\$ 446,694	\$ 453,246
TOTAL PLANT INVESTMENT	\$ 505,393	\$ 407,295	\$ 360,510	\$ 360,510		\$ 900,940

The water decomposition plant estimate is based on the process flow sheet adopted for this part of the study. Changes in the flow sheet, to be considered in Task III and as part of other studies, are expected to demonstrate even lower costs than those used here. Indirect costs were assumed as incremental factors to those used for the VHTR. The interest during construction considers an overall eight years program.

### 5.3.2 Comparison of Operating and Maintenance Costs

A summary comparison of annual operating and maintenance costs is shown in Table 5.3.2. Direct O&M costs are made up of payroll, consumable supplies and equipment and outside support services. Breakdowns and discussion on the various items within the direct O&M costs are shown in Section 4 of this report.

The annual cost of maintaining plant working capital is also part of the O&M costs, and the basis for the cost of working capital is shown in Table 5.3.3. Average net cash required was assumed to be 2.7 percent of the direct O&M costs, less nuclear liability insurance premiums. An approximately sixty day supply of consumable supplies, equipment, and coal was assumed to be on hand. The coal storage was evaluated at a cost of 2.2¢/kg (\$20/ton). The comparable fuel inventory charges for the nuclear fuel is traditionally considered part of the fuel cost and therefore was not included here.

### 5.3.3 Comparison of Fuel Costs

A comparison of the annual fuel costs from the four types of plants is shown in Table 5.3.4 for the base case. "Fuel" was defined, in this context, as all sources of energy needed by the processes.

For the water electrolysis plant, where large quantities of electric power are required, a large nuclear powerplant whose output is dedicated to the electrolysis plant would provide the lowest cost electric power. Therefore, electrolysis was based on the cost of power from a dedicated utility financed nuclear power station. The cost of power from this plant, as discussed in Section 4.2, is 1.28¢/kW-hr.

Coal gasification plants purchase power at an industrial rate from an electric utility at a cost of 2¢/KWH. This cost assumes that the power comes from a mix of nuclear and fossil sources and includes the cost of transmission as well as generation. Base coal costs of 2.2¢/Kg (\$20/ton) were assumed, which are representative of today's cost of deep mined coal.

The nuclear fuel costs from the VHTR are assumed to be 24.75¢/GJ (26.1¢/10<sup>6</sup> Btu), as reported in Reference 1. This cost does not represent an optimized fuel cost nor does it reflect the fuel reprocessing cost savings that are possible with the fuel design described in that reference. This cost can be compared with the 19.98¢/GJ (21¢/10<sup>6</sup> Btu) which represents fuel costs in today's light water reactors.

TABLE 5.3.2

TOTAL ANNUAL O&M COMPARISON  
(THOUSANDS OF DOLLARS)

	<u>ELECTROLYSIS</u>	<u>K - T</u>	<u>BI-GAS</u>	<u>WATER DECOMPOSITION</u>
DIRECT O&M COSTS	\$ 2,239	\$ 9,156	\$ 9,957	\$ 4,944
COST OF WORKING CAPITAL	<u>\$ 12</u>	<u>\$ 1,350</u>	<u>\$ 1,217</u>	<u>\$ 47</u>
TOTAL	\$ 2,251	\$ 10,506	\$ 11,174	\$ 4,991

TABLE 5.3.3

COMPARATIVE WORKING CAPITAL ESTIMATE  
(IN THOUSANDS OF DOLLARS)

	<u>ELECTROLYSIS</u>	<u>K - T</u>	<u>BI-GAS</u>	<u>WATER DECOMPOSITION</u>
AVERAGE NET CASH REQUIRED	\$ 60	\$ 247	\$ 269	\$ 123
MATERIALS & SUPPLIES IN INVENTORY				
CONSUMABLE SUPPLIES AND EQUIPMENT	\$ 63	\$ 555	\$ 670	\$ 155
COAL STORAGE	-	\$12,702	\$11,232	-
PRE-PAID NUCLEAR INS.	-	-	-	\$ 195
TOTAL WORKING CAPITAL	\$ 123	\$13,504	\$12,171	\$ 473
ANNUAL CHARGE RATE	10%	10%	10%	10%
ANNUAL COST OF WORKING CAPITAL	\$ 12	\$ 1,350	\$ 1,217	\$ 47

TABLE 5.3.4

ANNUAL "FUEL" COST COMPARISON  
(THOUSANDS OF DOLLARS)

	<u>ELECTROLYSIS</u>	<u>K - T</u>	<u>BI-GAS</u>	<u>WATER DECOMPOSITION</u>
ELECTRICITY				
UNIT COST	1.28¢/KWH	2¢/KWH	2¢/KWH	-
TOTAL COST	\$153,958	\$ 6,167	\$14,025	-
COAL				
UNIT COST	-	\$ 22/tonne	\$ 22/tonne	-
TOTAL COST	-	\$61,816	\$46,565	-
NUCLEAR				
UNIT COST	-	-	-	24.75¢/GJ
TOTAL COST	-	-	-	\$20,071
TOTAL "FUEL" COST	\$153,958	\$67,983	\$60,590	\$20,071



#### 5.3.4 Comparison of Hydrogen Production Costs

The base case hydrogen production costs are shown in Table 5.3.5. For the base case, the plants are assumed to be operating at an 80 percent capacity factor. The size of the plants is large enough to justify the centralized, or utility ownership, of the facility with the product distributed to any number of "consumers." The production costs, calculated on an annual basis, include a 10 percent charge on non-depreciating capital (land) and 15 percent annual charge on depreciating assets. The production cost includes profit, taxes, amortization, and other costs of business so that, in reality, the production cost is a "gate price" - the price at which hydrogen can be sold exclusive of the costs of transmission and distribution. The production costs indicated do not include any allowance for the sale of by-products, e.g., oxygen. If, for example, oxygen were sold instead of vented, then the cost of hydrogen would be reduced by about 1.7¢/std m<sup>3</sup> (42¢/10<sup>3</sup> SCF) if the oxygen credit were 2.2¢/Kg (\$20/ton).

The hydrogen production costs are plotted parametrically in Figure 5.3.1 to demonstrate visually the effects of fuel or coal cost on the gate price of hydrogen. Since neither the water electrolysis nor water decomposition costs depend directly on the cost of coal, they appear as horizontal lines in the figure. A range of nuclear fuel costs is included, however, to represent the changes in the economics of nuclear fuel in the future. From this comparison, it appears that the hydrogen from a water decomposition system, although higher in purity than that from coal gasification units, shows a competitive edge for coal costs that are frequently predicted for the near future. For example, the range of breakeven coal costs go from 99¢/GJ (\$1.0/10<sup>6</sup> Btu or about \$24/ton) for the base case nuclear water decomposition plant to about \$1.3/GJ (\$1.38/10<sup>6</sup> Btu, about \$33/ton) for a case with the nuclear fuel costs about twice as high as the base case. If an oxygen credit is assumed, then the break even coal cost reduces substantially.

While the base case comparison of production costs was predicated on an 80 percent capacity factor, it is important to recognize that capacity factor has a significant effect on the total economics of production. Figure 5.3.2 illustrates this effect. As can be seen, the shape of the curve depends upon the proportion of fixed and variable costs associated with production.

TABLE 5.3.5

HYDROGEN PRODUCTION COST COMPARISON  
(80% CAPACITY FACTOR, UTILITY OWNERSHIP)  
(THOUSANDS OF DOLLARS)

	COAL GASIFICATION			WATER DECOMPOSITION
	<u>ELECTROLYSIS</u>	<u>K - T</u>	<u>BI-GAS</u>	
<u>ANNUAL COSTS</u>				
NON-DEPRECIATING CAPITAL	\$ 80	\$ 100	\$ 100	\$ 100
DEPRECIATING CAPITAL	\$ 75,689	\$ 60,944	\$ 53,927	\$ 134,991
OPERATION AND MAINTENANCE	\$ 2,251	\$ 10,506	\$ 11,070	\$ 4,991
"FUEL"	\$ 153,958	\$ 67,983	\$ 60,590	\$ 20,071
TOTAL ANNUAL COST	\$ 231,978	\$ 139,533	\$ 125,687	\$ 160,153
<u>ANNUAL PRODUCTION</u>	2.74 x 10 <sup>9</sup> std m <sup>3</sup> (10.24 x 10 <sup>10</sup> SCF)	2.78 x 10 <sup>9</sup> std m <sup>3</sup> (1.042 x 10 <sup>11</sup> SCF)	2.82 std m <sup>3</sup> (1.05 x 10 <sup>11</sup> SCF)	2.86 x 10 <sup>9</sup> std m <sup>3</sup> (1.107 x 10 <sup>11</sup> SCF)
<u>PRODUCTION COST</u>	8.47¢/std m <sup>3</sup> (\$2.27/MSCF) \$6.62/GJ (\$6.98/10 <sup>6</sup> Btu)	5¢/std m <sup>3</sup> (\$1.34/MSCF) \$3.71/GJ (\$3.91/10 <sup>6</sup> Btu)	4.46¢/std m <sup>3</sup> (\$1.20/MSCF) (\$3.51/GJ) \$3.71/10 <sup>6</sup> Btu)	5.4¢/std m <sup>3</sup> (\$1.45/MSCF) \$4.22/GJ (\$4.45/10 <sup>6</sup> Btu)

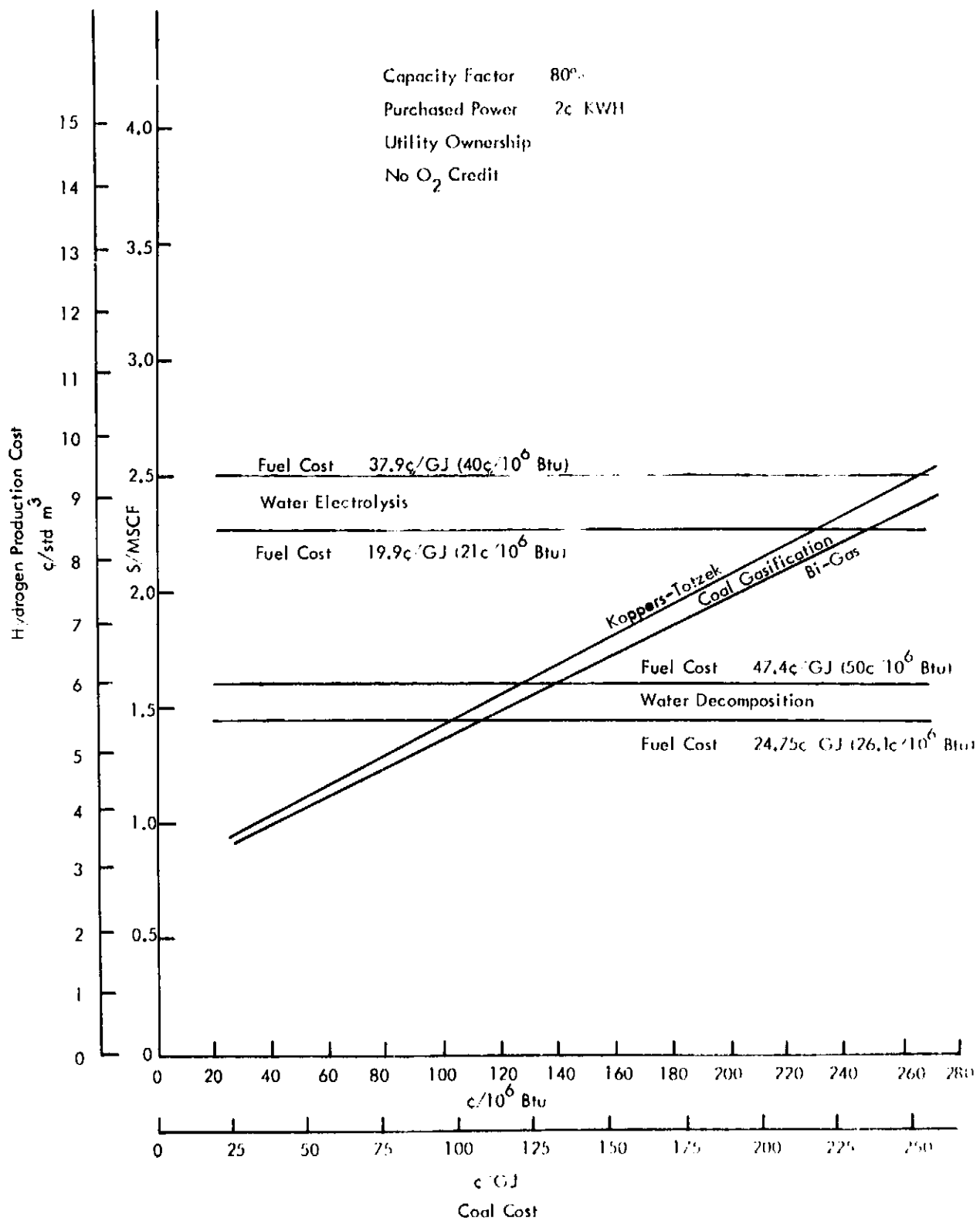


Figure 5.3.1 Comparative H<sub>2</sub> Production Cost

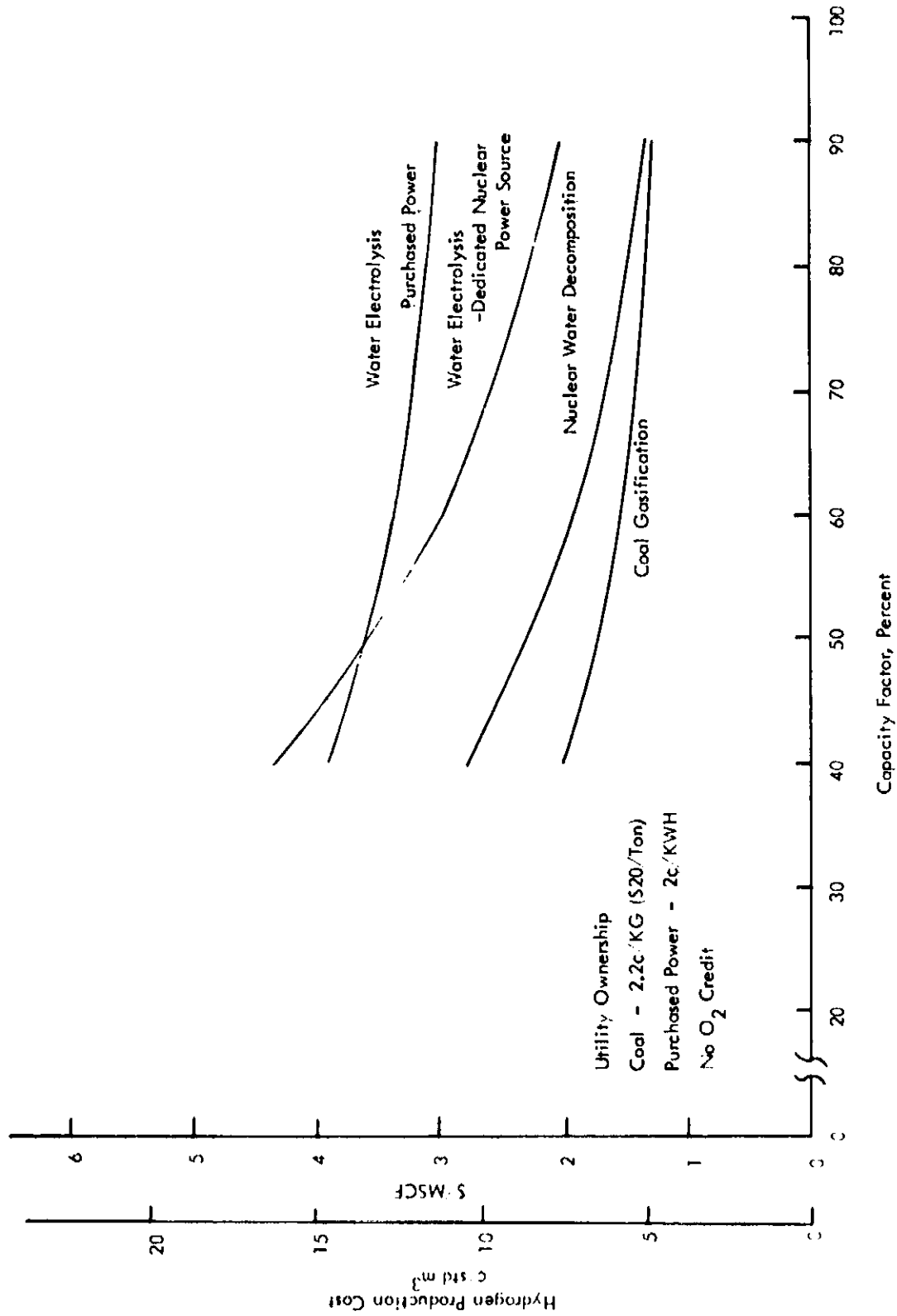


Figure 5.3.2 Sensitivity of H<sub>2</sub> Cost to Capacity Factor

#### 5.4 COMPARISON OF RESOURCE UTILIZATION AND ENVIRONMENTAL IMPACT POTENTIAL

The four hydrogen production processes can be compared on their relative utilization of resources and their relative potential for impacting the environment. These comparisons are made on a quantitative basis supplemented by inevitable subjective judgments.

Some perspective can be gained regarding the relative performance of the processes by examining the total energy inputs and outputs. This is done in Table 5.4.1. The process efficiencies are compared by converting inputs and outputs into equivalent heat units. For water electrolysis, the thermal energy required to generate the electrical requirements of the process is included and reduces the overall efficiency of water electrolysis to 28 percent. The efficiencies of the other systems are comparable and fall in the 46 to 49 percent range. It is emphasized that the 47 percent efficiency for the nuclear water decomposition process is a conservative figure based on the non-optimized flow diagram used in preparing the preliminary conceptual design and cost estimate.

In addition to energy inputs and outputs, it is instructive to examine, on an overall basis, the annual consumption of resources for each process. This comparison is shown in Table 5.4.2. The large water consumption for the electrolysis process comes from the inclusion of the evaporative loss of the cooling water for the nuclear reactors chosen to generate the power required for electrolysis. If a more efficient power generation cycle were assumed, the water consumption would reduce. The amount of uranium oxide required for power and/or process heat is also compared for all systems, assuming that nuclear power, using light water reactor for water electrolysis and coal gasification and the VHTR for water decomposition is used for all electric generation. Here again electrolysis requirements are greatest because of its relatively poor overall efficiency.

The water electrolysis and nuclear water decomposition processes produce oxygen as a by-product and a small amount of solid waste (resin, filtration residue, catalyst in the case of the nuclear water decomposition process, etc.) The coal processes yield carbon dioxide and a substantial amount of solid waste (ash, catalysts, sulfur, flue gas cleanup wastes, etc.) Differences in the coal processes are due to the use of a somewhat different coal for each process.

Considering the quality of the product hydrogen, a comparison of purity is shown in Table 5.4.3. The water electrolysis and nuclear water decomposition processes produce very high purity hydrogen. The use of 98 percent oxygen in the Koppers-Totzek process gives a lower quality hydrogen, but, because it contains 1.4 percent methane, it has the highest heating value. Bi-Gas hydrogen is purer than the Koppers-Totzek gas because of the use of purer oxygen and process modifications made to reform the large amount of methane formed in the gasifier.

TABLE 5.4.1

PROCESS EFFICIENCY COMPARISON

	<u>WATER ELECTROLYSIS</u>	<u>KOPPERS TOTZEK</u>	<u>BI-GAS</u>	<u>NUCLEAR WATER DECOMPOSITION</u>
HEAT INPUTS				
POWER, GJ/hr	18,130	440	1160	11,592
COAL, GJ/hr	-	10,504	10,015	-
TOTAL HEAT INPUT, GJ/hr	18,130	10,944	11,175	11,592
HEAT OUTPUTS				
PRODUCT GAS, std m <sup>3</sup> /hr	3.91 x 10 <sup>5</sup>	3.9 x 10 <sup>5</sup>	4.02 x 10 <sup>5</sup>	4.23 x 10 <sup>5</sup>
HEATING VALUE (WEIGHTED), MJ/std m <sup>3</sup>	12.79	13.48	12.71	12.79
TOTAL HEAT OUTPUT, GJ/hr	5008	5365	5108	5410
OVERALL PROCESS EFFICIENCY	27.6%	49.0%	45.7%	46.7%

TABLE 5.4.2

ANNUAL RESOURCE CONSUMPTION AND PROCESS OUTPUT

	<u>WATER ELECTROLYSIS</u>	<u>KOPPERS- TOTZEK</u>	<u>BI-GAS</u>	<u>NUCLEAR WATER DECOMPOSITION</u>
INPUT				
WATER, kg	$4.64 \times 10^{10}$	$2.0 \times 10^{10}$	$1.95 \times 10^{10}$	$1.95 \times 10^{10}$
COAL, kg	-	$2.8 \times 10^9$	$2.13 \times 10^9$	-
ELECTRICITY, kwh	$120 \times 10^8$	$3.1 \times 10^8$	$7.0 \times 10^8$	-
CATALYSTS/CHEMICALS, kg	$7.26 \times 10^4$	$1.1 \times 10^8$	$1.36 \times 10^8$	$4.35 \times 10^5$
URANIUM OXIDE ( $U_3O_8$ ), kg	$40.8 \times 10^4$	$9.07 \times 10^3$		$18.1 \times 10^4$
PROCESS OUTPUT				
PRODUCT GAS STREAM, std m <sup>3</sup>	$2.74 \times 10^9$	$2.79 \times 10^9$	$2.82 \times 10^9$	$2.96 \times 10^9$
BY-PRODUCTS OR WASTE				
OXYGEN, std m <sup>3</sup>	$1.37 \times 10^9$	-	-	$1.48 \times 10^9$
CARBON DIOXIDE, std m <sup>3</sup>	-	$1.85 \times 10^9$	$1.1 \times 10^9$	-
SOLIDS, kg	$6.8 \times 10^4$	$6.35 \times 10^8$	$4.99 \times 10^8$	$4.17 \times 10^5$

TABLE 5.4.3

HYDROGEN PRODUCT PURITY

	<u>WATER ELECTROLYSIS</u>	<u>KOPPERS- TOTZEK</u>	<u>BI-GAS</u>	<u>NUCLEAR WATER DECOMPOSITION</u>
HYDROGEN, %	99.9	95.4	99.3	99.9
NITROGEN, %	TRACE	1.4	0.7	NIL
METHANE, %	NIL	3.2	NIL	NIL



As part of the comparative evaluation, an assessment of environmental areas of concern was made. The major areas of potential impact included: air quality, water quality, solid waste, land use, water use, fuel use, noise, aesthetics, and socio economic factors. It was assumed that all four processes could be engineered to meet applicable federal and state regulations and standards. After quantifying the environmental impact potential for the four processes, it was concluded that all should have an acceptable level of impact on the environment.

In evaluating the potential impact of processes on air and water quality and use, designing to meet applicable standards dictates that the impact will be felt ultimately on the economics of the plant rather than on the environment. Thus designing plants with cooling towers, flue gas cleanup devices, etc. will increase plant complexity while avoiding environmental deterioration.

With respect to production of solid wastes, an analogy is seen with present generation electric power plants - nuclear and fossil. While coal fired plants require provision for disposal of solid products of combustion, e. g. ash, nuclear plants involve a long range consideration of radioactive waste disposal. (Both types of plants are presently inherent in our utility baseload structure). Again it was assumed that all four types of plants can be engineered to meet applicable regulations and standards.

Any change in the physical or social environment has an effect (impact) on that environment even if the impact is acceptable. Even when standards are met, emissions and discharges can contribute to mankind's accumulative impact on his environment and can be rated in terms of their magnitude. An impact may be good or bad depending on viewpoint and location. For example, a new industry in a location with a labor surplus or housing surplus would have a beneficial sociocultural impact. If located in a very small community, the resulting influx of workers and their families would put stress on public services which would be viewed by most as an adverse impact.

Comparing processes is simple when there is a common denominator such as the number of employees, but if there is no common denominator it becomes a value judgment. Primary impacts in this case are those which are regulated by law or are effected by local or national policies. These have been recognized as important to enough people that political action has been taken. Secondary impacts are extremely local and effect only a few people as a result of the location of the proposed production. The choice of "Middletown," population 250,000, as a site negates sociocultural impacts which might be expected in a smaller community.

In view of the designs and assumptions made in this study, the processes were compared in terms of each potential impact and ranked. A rating of 0 denotes no impact, -1 denotes a slightly adverse impact and a -10 denotes a large impact potential while still meeting standard guidelines. The rankings are summarized in Table 5.4.4, "Environmental Impact Potential."

TABLE 5.4.4  
ENVIRONMENTAL IMPACT POTENTIAL

	<u>Electrolysis</u>	<u>K - T</u>	<u>Bi-Gas</u>	<u>Nuclear Water Decomposition</u>
<u>Primary Impacts</u>				
Air quality	-2	-4	-3	-1
Water quality	-2	-3	-2	-1
Solid waste	-5	-7	-6	-4
Land use	-4	-1	-1	-2
Water use	-5	-2	-2	-2
Fuel use	<u>-5</u>	<u>-3</u>	<u>-2</u>	<u>-1</u>
Sub Total	-23	-20	-16	-11
<u>Secondary Impacts</u>				
Noise	-1	-3	-3	-2
Aesthetics	<u>-1</u>	<u>-3</u>	<u>-3</u>	<u>-2</u>
Sub Total	-2	-6	-6	-4

In terms of air quality, the coal gasification processes rated lowest due to emissions of the products of the combustion of coal. The K-T process was lower because it consumes more coal than the Bi-Gas process.

Water vapor emissions, due to heat dissipation requirements, account for electrolysis being rated lower than nuclear water decomposition, in respect to water quality, because it involved a larger reactor and about twice as much heat dissipation. The large cooling system needed for the electrolysis power plant also increases the potential for water quality impacts through increased blowdown and entrainment of organisms at the intake. Coal storage and handling facilities involve potential water quality hazards through runoff and sludge. The potential impact is assigned to the coal gasification processes in relation to their relative coal consumption.

Solid wastes generated by the processes are assumed to be disposed of by environmentally sound means and therefore their impact is in indirect relation to their quantity.

Land use represents another direct relationship between requirement and impact. The rankings for land use shown in Table 5.4.4 were based on estimates of land required by the plants.

Middletown, the site basis for the assessment, has an ample supply of water and fuel. Therefore the consumption of these resources is more of a national concern than a local concern. The actual chemical use of water is in all cases relatively small. The use of water for cooling is large and in direct relation to heat dissipated because all plants use cooling towers. Therefore, electrolysis, which is only half as efficient, is by far the largest consumer of water and fuel. The coal gasification processes are penalized because alternative uses of coal increase its value as a resource.

Noise and aesthetics favor electrolysis because it has a low profile and a large exclusion area. Nuclear water decomposition also has the benefit of an exclusion zone. The coal gasification processes receive lower ratings in this area because they do not have exclusion zones and involve multi-story facilities, the noise of coal handling, and on-site coal storage.

Nuclear water decomposition was ranked best in terms of minimum potential environmental impact. The K-T Process was ranked slightly below the Bi-Gas Process due mostly to its greater coal consumption. The major drawback to electrolysis was the inherent weakness in its overall process efficiency. It should be stressed that these rankings are subjective and relative and do not imply that any of the processes cannot meet the environmental standards that are foreseen for the future.

## 6.0 SUMMARY OF RESULTS

The scope of work called for in Tasks I and II of the "Studies of the Use of Heat From High Temperature Nuclear Sources for Hydrogen Production Processes", reported herein, requires that:

- A projection be made of the potential market for hydrogen as a fuel and feedstock through the year 2000.
- Processes for the production of hydrogen be selected from among water electrolysis, fossil based (steam hydrocarbon), and thermochemical water decomposition systems and be evaluated in terms of relative performance, economics, resource requirements, and technology status.

The results of the Task I and II effort are summarized below.

### 6.1 HYDROGEN MARKET PROJECTION

The study considered both the total potential market for hydrogen and the part of that market that might be captured by nuclear driven thermochemical water decomposition plants. The latter becomes important in assessing the need for, and justification for, the development of high temperature nuclear heat sources and thermochemical hydrogen production processes.

The United States currently uses about  $8 \times 10^{10}$  standard cubic meters ( $3 \times 10^{12}$  SCF) of hydrogen per year. Production is growing today at a rate of 6 percent per year, and is expected to grow even more rapidly in the future. The projection made here predicts a base case hydrogen requirement, to the year 2000, of  $1.3 \times 10^{12}$  std  $m^3$  per year ( $4.8 \times 10^{13}$  SCF per year). The range of hydrogen consumption, about the base, goes from a low estimate of  $6.4 \times 10^{11}$  std  $m^3$  per year to a high of  $1.7 \times 10^{12}$  std  $m^3$ /year. Predictions by others range from  $3.5 \times 10^{11}$  to  $1.7 \times 10^{12}$  std  $m^3$ /year. It should be noted that if the market continues to grow at its present six percent per year, the year 2000 demand for hydrogen would be about  $4 \times 10^{11}$  std  $m^3$ /year ( $1.5 \times 10^{13}$  SCF/year).

The largest potential market foreseen for hydrogen is in the production of substitute natural gas (SNG) and synthetic oils from coal. The markets for hydrogen use in oil refineries and chemical processes, e.g., ammonia and fertilizer production, is smaller but still significantly large. The demand for hydrogen for direct-reduction iron-making is seen to be relatively small, primarily because of the slow growth projected for the United States steel industry. Hydrogen for use as a fuel will be but a limited market. Its application to aircraft appears to have real promise and will constitute the bulk of the hydrogen fuel market. Other direct fuel needs are expected to be met, in the main, by nuclear, coal, and synthetic fuels. This last requires, of course, hydrogen as a feedstock.

The ability of nuclear water decomposition systems to participate in the growing hydrogen market is dependent upon when these systems are available and whether their economics permits reasonable penetration of the available market. A base case estimate considers that the very high temperature nuclear heat source, and the hydrogen production process, are both commercially available in 1995. It is further assumed that, upon introduction, the nuclear hydrogen system can penetrate the newly committed production capability at a rate of 10 percent per year for all markets except hydrogen fuel and five percent per year for the direct fuel market. With these assumptions, there would be required, by the year 2000, approximately 15-30 nuclear hydrogen generating systems with nominal ratings of  $9.6 \times 10^6$  std cubic meters per day ( $360 \times 10^6$  SCFD) each.

## 6.2 HYDROGEN PRODUCTION PROCESSES

The hydrogen production processes selected for evaluation were:

- Water electrolysis, using the Teledyne HP electrolyzer modules
- Coal gasification, using the Bi-Gas two stage pressurized gasifier to represent developing coal gasification technology
- Coal gasification, using the Koppers-Totzek atmospheric gasifier to represent commercially available coal gasification technology.
- Water decomposition, using the Westinghouse Sulfur Cycle thermochemical hydrogen production process in combination with a very high temperature nuclear reactor (VHTR) heat source

### 6.2.1 Water Electrolysis

The technology of water electrolysis is well known. Water electrolyzers are available commercially from many manufacturers. The preliminary conceptual design used for evaluation purposes, based on the use of Teledyne HP electrolyzer modules, was a complete hydrogen generation facility producing  $9.4 \times 10^6$  std cubic meters/day ( $351 \times 10^6$  SCFD) of 99.9% pure hydrogen at a delivery pressure of 6895 kPa (1000 psi). The thermal efficiency of the electrolysis plant is 81 percent, not including the efficiency of producing the electric power required for the process. When the electric generation efficiency is included at 34 percent, typical of the light water nuclear reactor powerplants capable of producing the lowest cost electric power currently available, the combined overall process efficiency drops to 28 percent. The cost of producing hydrogen from this plant, based on utility ownership and costs in effect in mid-1974, is estimated to be approximately 8.47¢/std m<sup>3</sup> (\$2.27/MSCF) when operating at an 80 percent capacity factor and supplied with power from an adjacent nuclear power station with a fuel cost of 19.9¢/GJ (21¢/10<sup>6</sup> Btu), as shown in Figure 6.2.1.

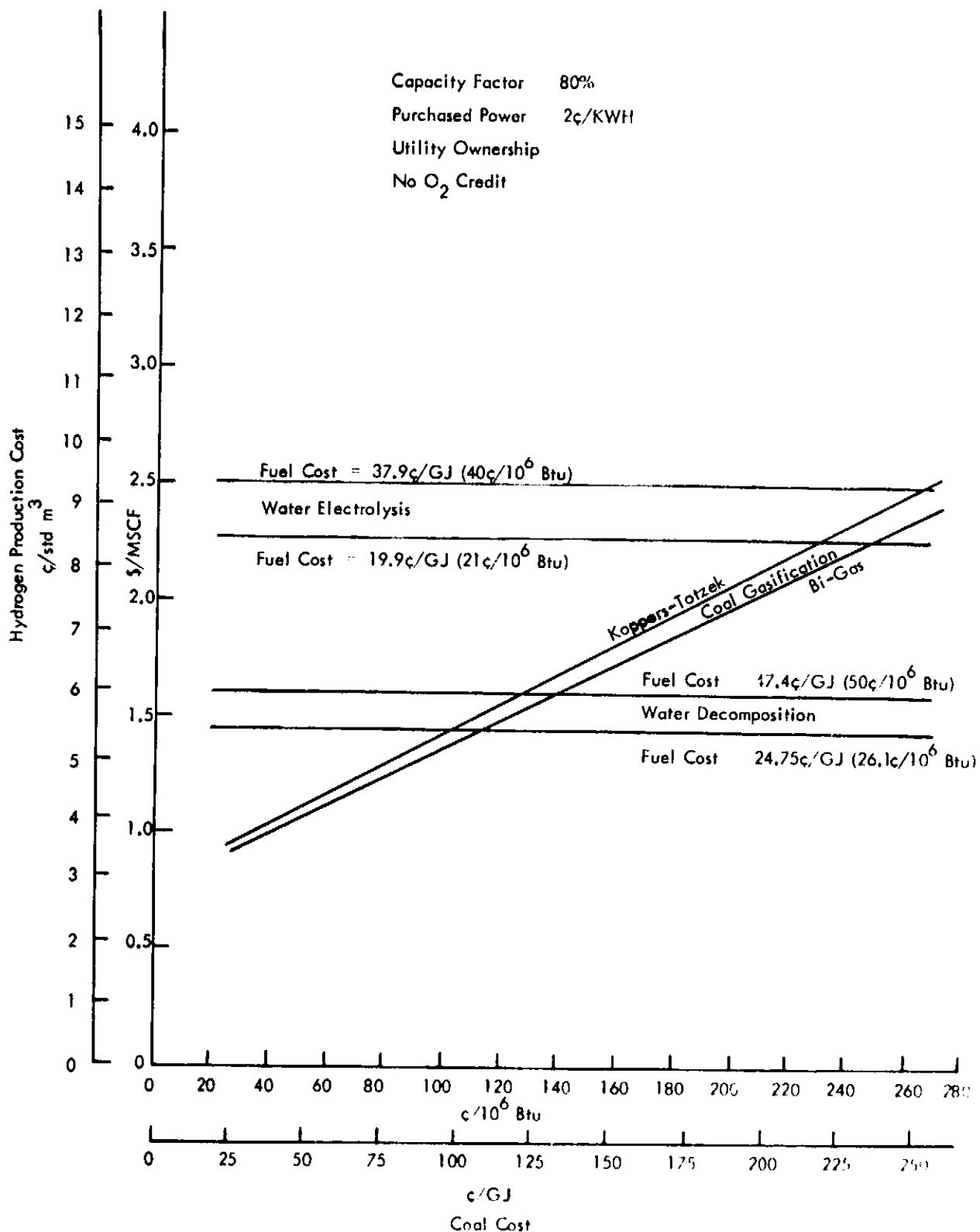


Figure 6.2.1 Comparative H<sub>2</sub> Production Cost

### 6.2.2 Bi-Gas Coal Gasification

The Bi-Gas gasifier is a two stage pressurized system which represents developing technology in coal gasification. A pilot plant using this type of gasifier is scheduled for initial operation in 1975. The pilot plant should confirm the characteristics of the gasifier and lead to commercialization of the system. The Bi-Gas system, operating at a pressure of 6895 kPa (1000 psi), tends to favor the production of methane. For the evaluation, therefore, downstream processing was incorporated to separate the methane from the hydrogen, reform the methane to hydrogen and carbon monoxide, shift the carbon monoxide to hydrogen and carbon dioxide, and remove the carbon dioxide. In this manner, a single product stream of  $9.65 \times 10^6$  std  $m^3$ /day ( $360 \times 10^6$  SCFD) of 99.3 percent pure hydrogen could be produced. The overall thermal efficiency of the plant, relating the higher heating value of the product gas to the total energy input to the plant, was calculated to be 46 percent. The cost of the production facility included, as in all the processes, equipment and facilities, such as cooling towers and flue gas cleanup systems, to assure that the plants would meet the appropriate environmental standards and regulations. The cost of producing hydrogen from this plant, under base case economic conditions, is 4.46¢/std  $m^3$  (\$1.20/MSCF). The base case considered utility ownership, mid-1974 capital costs, an 80 percent capacity factor and coal at 2.2¢/kg (\$20/ton). The sensitivity of hydrogen production cost to the cost of coal is shown in Figure 6.2.1.

### 6.2.3 Koppers-Totzek Coal Gasification

Koppers-Totzek gasification is a commercially available process. Gasification plants using these gasifiers are in existence around the world. The gasifier, which operates at approximately atmospheric pressure, can handle any kind of coal and, with appropriate downstream processing, produce a hydrogen product stream. The plant design considered for the evaluation used ten four headed gasifiers to produce a synthesis gas that was further processed by acid gas removal, carbon monoxide shift conversion, carbon dioxide removal, and polishing methanation to produce  $9.56 \times 10^6$  std  $m^3$ /day ( $357 \times 10^6$  SCFD) of a gas containing 95.4 percent hydrogen by volume. Compression stages were included in the processing steps to result in the product gas being available at a pressure of 6895 kPa (1000 psi) for off-site distribution. The overall thermal efficiency of the process, including the energy consumed in gas compression and other plant services, is evaluated to be 49 percent. The base economic evaluation, using mid-1974 costs, utility ownership, an 80 percent capacity factor, and a delivered coal cost of 2.2¢/kg (\$20/ton), resulted in a hydrogen production cost of 5¢/std  $m^3$  (\$1.34/MSCF). Figure 6.2.1 shows the sensitivity of the cost of producing hydrogen to the cost of coal.

### 6.2.4 Nuclear Water Decomposition

The water decomposition system used for evaluation is the Westinghouse Sulfur Cycle two-step thermochemical process. In this process, hydrogen and sulfuric acid are produced electrolytically by the reaction of sulfur dioxide and water. The process is completed by

vaporizing the sulfuric acid and thermally reducing, at higher temperatures, the resultant sulfur trioxide into sulfur dioxide and oxygen. Following separation, sulfur dioxide is recycled to the electrolyzer and oxygen is either vented or sold.

As in conventional water electrolysis, hydrogen is produced at the electrolyzer cathode. Unlike water electrolysis, sulfuric acid, rather than oxygen, is produced at the anode. Operation in this fashion reduces the theoretical power required per unit of hydrogen production by more than 85 percent over that required in water electrolysis. This is partially offset, however, by the need to add thermal energy to the process in the acid vaporizer and the sulfur trioxide reduction reactor. Even so, by avoiding the high overvoltages at the oxygen electrode of a conventional electrolyzer, as well as the inefficiencies associated with power generation, this hydrogen generation process provides overall thermal efficiencies approximately double those attainable by conventional electrolytic hydrogen and oxygen production technology.

The energy source for the water decomposition system is a very high temperature nuclear reactor (VHTR) producing both electric power and a high temperature helium stream to the process. The VHTR is a graphite moderated helium cooled nuclear unit that is predicated on the integration of the technologies from the NERVA nuclear rocket engine program and land based gas cooled reactor programs into an advanced very high temperature nuclear heat and power source.

The integrated plant requires, for the process flow sheet adopted for this initial iteration of the conceptual design, a VHTR rated at 3220 MW(t) to result in the production of  $10.1 \times 10^6$  standard cubic meters/day ( $379 \times 10^6$  SCFD) of 99.9 percent pure hydrogen. The VHTR provides all of the energy - heat and electricity - required for the operation of the water decomposition plant and for the auxiliary power requirements of the nuclear system. The overall thermal efficiency of the integrated process is calculated, for the present process configuration, to be 47 percent for the system producing hydrogen for off-site consumption at a pressure of 6895 kPa (1000 psi).

The nuclear system and the water decomposition system both require a significant development effort to reach first large scale demonstration. The recommended program for the VHTR was determined as part of the VHTR effort supported by ERDA and reported in Reference 1. The development effort on the water decomposition system has, to date, been privately funded and has verified, by laboratory testing, that the electrolytic and chemical reactions proceed as written and at rates sufficient to insure an efficient and economic hydrogen production plant. The overall development program leading to commercialization of the process will be defined as part of the Task III effort.

Using the costs of the VHTR as determined in the ERDA sponsored program, adjusted to interface with the water decomposition plant requirements as developed in this study, in conjunction with the costs of the hydrogen production plant resulting from the study, the projected cost of hydrogen from a nuclear water decomposition plant was determined. For the



base economic case, i.e., 80 percent capacity factor, mid-1974 cost basis, utility ownership, nuclear fuel costs of 24.75¢/GJ (26.1¢/10<sup>6</sup> Btu), and no credit for the oxygen produced in the process, the hydrogen production cost, as shown in Figure 6.2.1, is 5.4¢/std m<sup>3</sup> (\$1.45/MSCF). The effects of varying fuel costs are also shown in the figure.

### 6.3 CONCLUSIONS

There is a market for hydrogen that exists today that is being met primarily by fossil based hydrogen generation processes. This market is expected to grow substantially over the next several decades. Simultaneously, the growing unavailability and/or escalating costs of the fossil feedstocks used in today's hydrogen production makes imperative the development of alternative hydrogen generation systems. These systems must make use of our most plentiful resources, i.e., they must be nuclear or coal based systems.

The evaluation of the nuclear water decomposition system, using the Sulfur Cycle, indicates that it is superior to water electrolysis in both thermal efficiency and cost of hydrogen produced regardless of whether the water electrolysis plant is powered by nuclear-electric or fossil-electric plants. Nuclear water decomposition is on a par with coal gasification systems in respect to thermal efficiency and holds great promise of lower hydrogen production costs as reasonable extrapolations of future nuclear and coal costs are made. The nuclear water decomposition system has a lower potential environmental impact than other systems. It also provides the opportunity for more effective resource management, such as making possible the utilization of all the carbon in coal for its chemical value, as opposed to converting it to carbon dioxide while extracting only its thermal value.

It is concluded that the nuclear water decomposition system shows sufficient technological and economic promise to warrant aggressive development of the process, and further definition of the conceptual design.

## APPENDIX A

### MATERIALS FOR THE SULFUR CYCLE WATER DECOMPOSITION SYSTEM

A materials investigation has been performed to determine unique or unusual materials requirements for the Sulfur Cycle water decomposition system. It has been determined that the critical problem areas involve the high temperature sulfuric acid loop shown in Figure 1. The remainder of the system operates at relatively low temperatures,  $< 476\text{K}$  ( $< 400^\circ\text{F}$ ) and thus can utilize commercially available components. The high temperature acid decomposition loop, because of the temperatures and pressures involved, departs significantly from standard sulfuric acid handling practice.

The acid decomposition process is carried out in the four successive steps involving four heat exchangers shown in Figure 1. Sulfuric acid at a concentration of 80 percent by weight is regeneratively heated from 433 to 725K (320 to 845 $^\circ\text{F}$ ) in E-1 and AV-1. In the remaining two units, AV-2 and DR-1, the process stream is heated by externally supplied heat from 725 to 1144K (845 to 1600 $^\circ\text{F}$ ).  $\text{SO}_3$  is thermally decomposed to  $\text{SO}_2$  and oxygen, with the aid of a catalyst, in DR-1. In each step, a severe burden is placed on structural materials. As indicated in the process flow diagram, sulfuric acid, 80 percent by weight, is converted into the gaseous state by boiling. The system pressure of 2069 kPa (300 psia) raises the boiling point to 593K (608 $^\circ\text{F}$ ). The most severe corrosion potential is expected to exist at the liquid - gas interface under both boiling and condensing conditions. Boiling is expected to occur in the acid vaporizer AV-1 where water is driven off as steam and the remaining acid increases in concentration to 100 percent before vaporizing to 725K (845 $^\circ\text{F}$ ). In the reduction reactor, DR-1, only gaseous products and reactants are present, consisting of superheated steam,  $\text{SO}_3$ ,  $\text{SO}_2$  and oxygen. In the return or secondary side of AV-1, heat is extracted reducing the product gas temperature from 1144 to 630K (1600 to 675 $^\circ\text{F}$ ). In this temperature range  $\text{H}_2\text{SO}_4$  begins to condense at a concentration near 100 percent by weight. In the economizer, E-1, more heat is removed resulting in further condensation and dilution of sulfuric acid. Products emerging from the economizer, E-1, are sulfuric acid at 80 percent concentration, superheated steam,  $\text{SO}_2$  and oxygen.

#### Material Considerations

The compatibility of the most common structural materials for sulfuric acid service is summarized in Table 1. The data are given for various acid concentration with upper temperature limits noted. In those cases where the boiling point is indicated, it is assumed to be one atmosphere. Of the materials which appear in the table, only a few are suitable for use with acid at concentrations above 80 percent. Temperature limitations reduce the number of candidate materials even further. The materials with the highest probability of surviving the conditions encountered in the sulfur cycle water decomposition cycle are listed below, along with comments concerning suitability with respect to requirements listed previously.

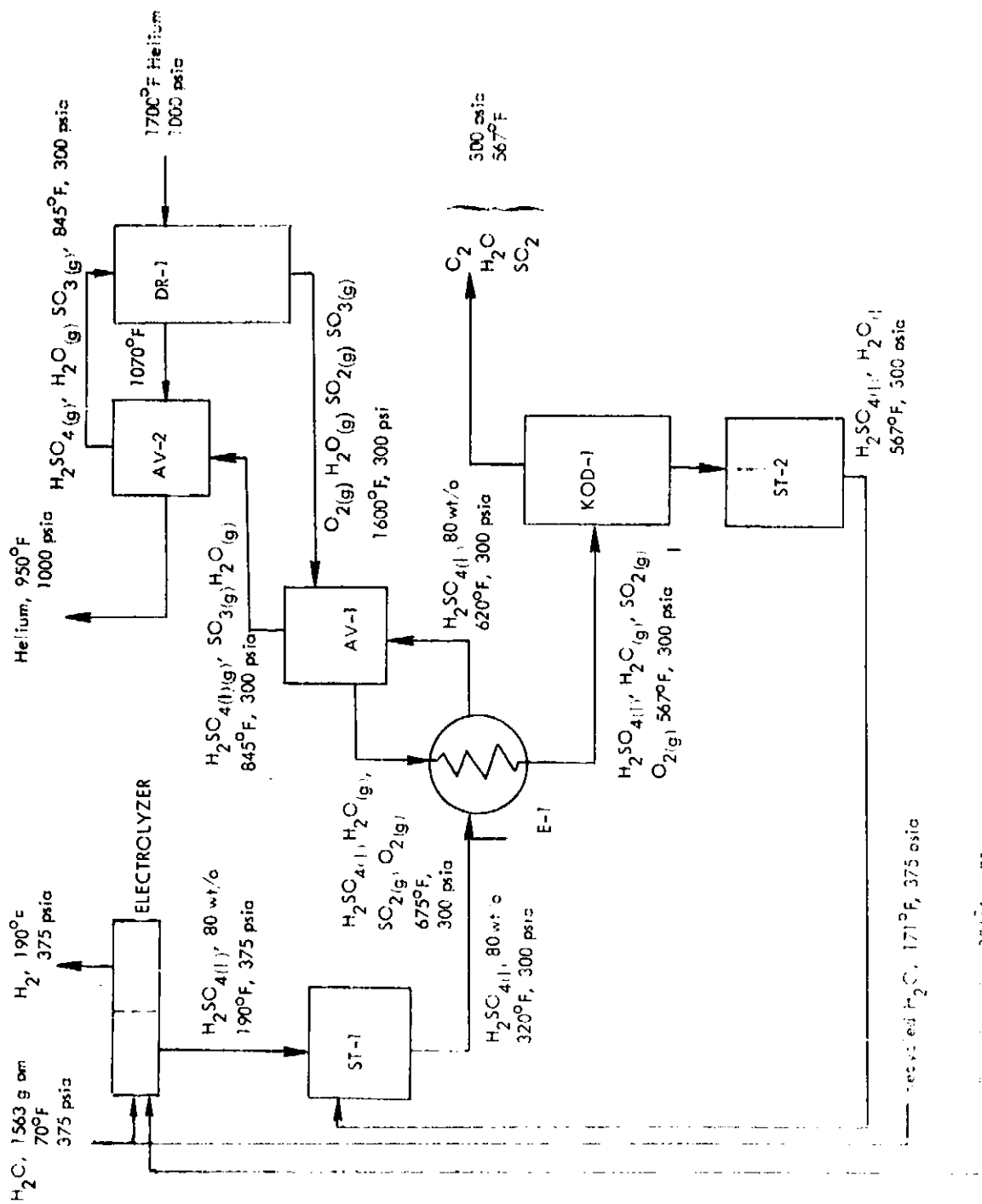


Figure 1. High Temperature Sulfuric Acid Loop

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TABLE 1

MATERIALS OF CONSTRUCTION FOR SULFURIC ACID AND  
OLEUM HANDLING (REFERENCE 39)

MATERIALS	0-10% H <sub>2</sub> SO <sub>4</sub>	10-50% H <sub>2</sub> SO <sub>4</sub>	50-60% H <sub>2</sub> SO <sub>4</sub>	60-75% H <sub>2</sub> SO <sub>4</sub>	75-90% H <sub>2</sub> SO <sub>4</sub> (includes 60° acid)	90-98% H <sub>2</sub> SO <sub>4</sub> (includes 66° acid)	98-100% H <sub>2</sub> SO <sub>4</sub>
Cast iron					to 175°F	to 225°F	
Platinum, gold or gold-platinum alloys	to b.p.	to b.p.	to b.p.	to b.p.	to b.p.	to b.p.	to b.p.
Lead or lead lining	to b.p.	to 400°F	to 400°F	to 400°F	to 85%, 350°F; to 90%, 250°F	to 96%, 140°F	
High silicon cast iron (Duriron)	to b.p.	to b.p.	to b.p.	to b.p.	to b.p.	to b.p.	to b.p.
DURIMET 20	to b.p.	to 176°F	to 176°F	to 150°F	to 150°F	to 176°F	to 176°F
CHLORIMET 2 or 3	2 to b.p. 3 to b.p.	2 to b.p. <sub>g</sub> 3 to 200°F	2 to b.p. <sub>g</sub> 3 to 200°F	2 to 250°F 3 to 175°F	2 to 250°F 3 to 175°F	2 to 250°F 3 to 225°F	2 to 250°F 3 to 250°F
Glass lined steel (avoid thermal shock)	to 500°F	to 500°F	to 500°F	to 500°F	to 500°F	to 176°F	to 500°F
HASTELLOY ALLOYS B-C-D-F	B to b.p. C to b.p. D to b.p. <sub>g</sub> F to 150°F	B to b.p. <sub>g</sub> C to 200°F D to b.p. <sub>g</sub> F to 150°F	B to b.p. <sub>g</sub> C to 200°F D to b.p. <sub>g</sub> F to 150°F	B to 250°F C to 175°F D to b.p. F not recommended	B to 250°F C to 175°F D to b.p. F not recommended	B to 300°F C to 200°F D to b.p. F not recommended	B to 300°F C to 200°F D to b.p. F not recommended
WORTHITE	to b.p.	to 175°F	to 150°F	to 140°F	to 140°F	93% to 150°F 98% to 175°F	to 175°F
Stainless steel type 316 and 317	to 5% belgw 150°F						
Carpenter Stainless 20Cb-3	to 5% belgw 250°F						

TABLE 1  
MATERIALS OF CONSTRUCTION FOR SULFURIC ACID AND  
OLEUM HANDLING (CONTINUED)

MATERIALS	0-10% H <sub>2</sub> SO <sub>4</sub>	10-50% H <sub>2</sub> SO <sub>4</sub>	50-60% H <sub>2</sub> SO <sub>4</sub>	60-75% H <sub>2</sub> SO <sub>4</sub>	75-90% H <sub>2</sub> SO <sub>4</sub> (includes 60° acid)	90-98% H <sub>2</sub> SO <sub>4</sub> (includes 66° acid)	98-100% H <sub>2</sub> SO <sub>4</sub>
Rubber or neoprene lined steel	to 150°F	to 150°F					
Special hard rubber lined steel	to 200°F	to 200°F					
Butyl rubber lined steel	to 200°F	to 200°F	to 150°F				
Carbon and graphite	to 340°F	to 340°F	to 340°F	to 340°F	to 340°F	to 96%, 340°F	
MONEL, copper, 10% alum. bronze	to 200°F in absence of oxygen	to 200°F in absence of oxygen	to 200°F in absence of oxygen				
Tantalum (avoid fluoride contaminated acid)	to b.p.	to b.p.	to b.p.	to b.p.	to 375°F	to 375°F	to 375°F
HERESITE	to b.p.	to b.p. up to 35% to 150°F over 35%	to 150°F	to 150°F	to 150°F	to 150°F	to 150°F
Fluoropolymers (Teflon, Kynar)	to 400°F	to 400°F	to 400°F	to 400°F	to 400°F	to 400°F	to 400°F
KOROSEAL	to 140°F	to 140°F					
Cypress or redwood	to 190°F						
HAVEG 41	to 300°F	to 300°F	to 240°F	to 205°F	to 150°F		
ILLIUM G, 98 and R	G to b.p. 98 to b.p. R to b.p.	G to 195°F above 40%, to b.p. below 40%; 98 to b.p.; R to b.p.	G to 195°F 98 to b.p. R to b.p.	G to 140°F 98 to 195°F R to 180°F	G for 75-80% to 140°F, for 80-85% to 195°F; 98 to 195°F; R to 180°F	G to 195°F 98 to 225°F R to 180°F	G to 195°F 98 to 225°F R to 180°F
Acid Proof Brick	to 600°F	to 600°F	to 600°F	to 600°F	to 600°F	to 600°F	to 600°F

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### Precious Metals

Gold, platinum and their alloys are noted for their resistance to acid attack to very high temperatures (Reference 40). Their cost restricts their use to thin clads on less expensive substrates. The use of precious metals in the water decomposition system is not considered because of the associated economic burden.

### Tantalum and Its Alloys

The use of this refractory metal in acid service is increasing. At acid concentrations below 80 percent and temperatures below 464K (375°F), the excellent corrosion resistances more than offset the relatively high cost of this material. However, at acid concentrations above 80 percent tantalum has a tendency to become embrittled due to hydrogen pickup. Tantalum also reacts with  $\text{SO}_3$  and  $\text{O}_2$  temperatures above 472K (400°F), limiting its use to lower temperatures.

### Alloys with High Silicon Content

Metallic alloys with high silicon content, such as Hastelloy D, Duriron, Durimet, and Chlorimet, are the standard structural materials used in the sulfuric acid industry today (References 39, 41). These materials are primarily casting alloys which are brittle, not readily joined by welding and are also notch sensitive. Consequently these materials are not normally utilized in a structural load-bearing capacity.

The effect of silicon content on the corrosion resistance of iron and steel is illustrated in Figures 2 and 3. In Figure 2, the corrosion rate of steel is shown as a function of acid concentration for a number of temperatures. In Figure 3, the corrosion behavior of Duriron, a cast iron with approximately 15 percent silicon, is shown at the boiling temperature as a function of acid concentration. A corrosion rate of 0.127 mm (5 mils) per year is indicated at the boiling point for concentrations above 80 percent. This corrosion rate is lowest for any non-precious metal. The effect of higher temperatures due to higher system pressure and the resulting increase in boiling point of the acid must be investigated.

### Glass and Glass Lined Steel

Glass or glass lined steel is commonly used for handling acid in the chemical industry. The behavior of glass in contact with sulfuric acid at various concentrations is shown in Figure 4 as a function of temperature (Reference 43). Above 80 percent concentration, glass is not resistant to attack at the acid boiling point. The reason for this behavior is shown in Figure 5 which shows the effect of superheated water on the corrosion of Pyrex glass. As the temperature increases above 422K (400°F), the silica in the glass becomes hydrated forming,  $\text{H}_2\text{SiO}_3$ , which is soluble in superheated water. Thus, the incompatibility is not with sulfuric acid, but with water, a decomposition product. Pyrex, according to

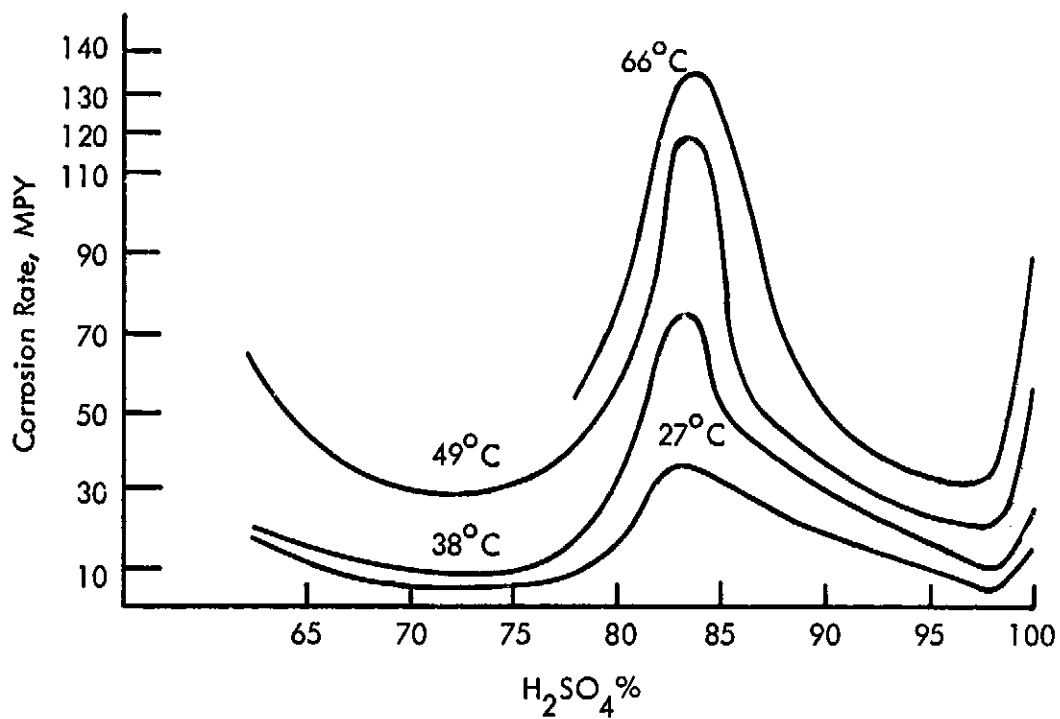


Figure 2. Corrosion of Steel by Sulfuric Acid, General Chemical Data  
(Reference 42)

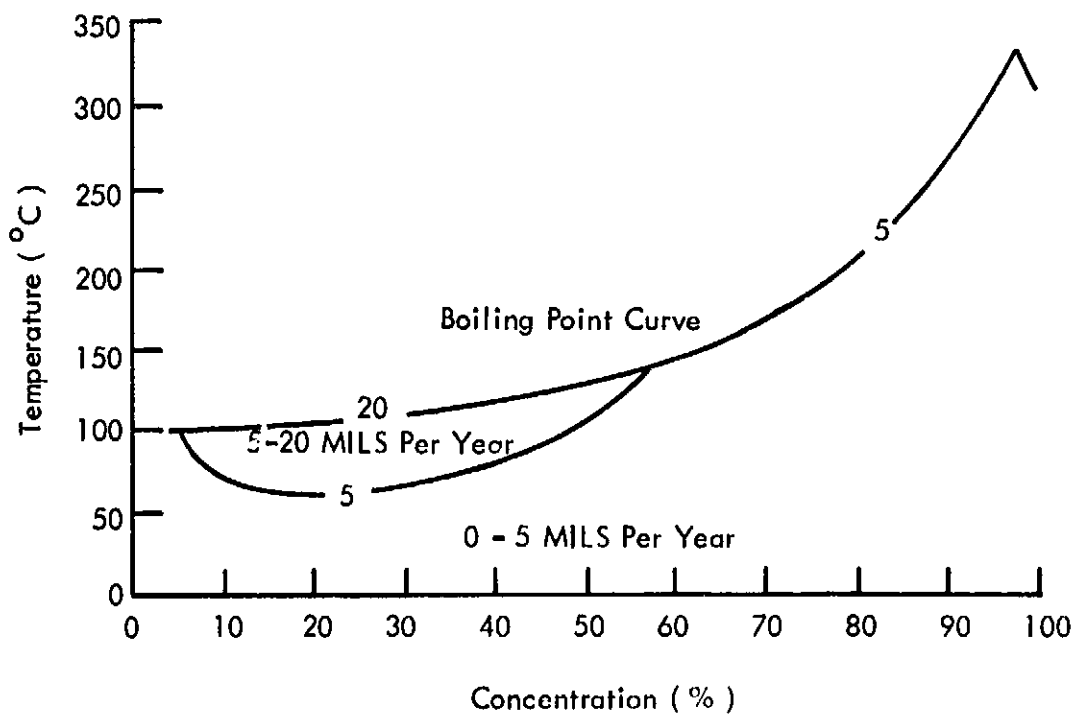


Figure 3. Corrosion Rate of Duriron in Sulfuric Acid  
(Reference 42)

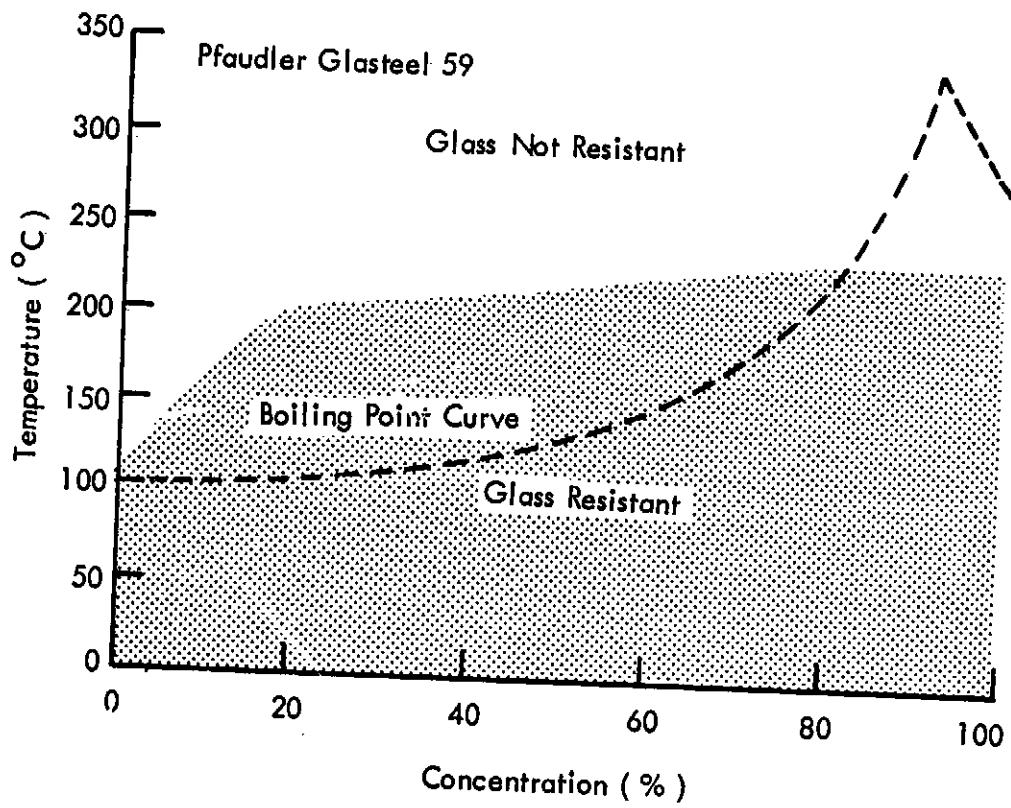


Figure 4. Corrosion Rate of Glass-Lined Steel in Sulfuric Acid  
(Reference 42)



Corning, is their most corrosion resistant glass. As indicated by the curve in Figure 5, the corrosion rate approaches 0.76 cm per year (0.3 inch per year) as the temperature nears 478K (400°F) and presumably continues to increase above 478K (400°F). This corrosion rate is unacceptable for long time applications.

#### Fluoropolymers (Teflon, Kynar)

Polymers such as Teflon exhibit excellent resistance to acid attack at all concentrations up to 478K (400°F) where thermal decomposition begins to occur. Polymers are used as liners on structural materials where loads are encountered, Reference 42.

#### Acid Proof Brick

Acid proof brick is the most widely used non-metallic material for construction of sulfuric acid plants (Reference 42). The bricks are used to line carbon steel shells. The lining serve to reduce temperatures at the surface of the metallic vessel. The brick linings are usually backed-up by a polymer or asphaltic mastic to protect the metallic liner from acid seepage through the brick-work. Recent advances in mortars have helped in overcoming swelling, a problem encountered in mist acid conditions or where frequent filling and emptying occurs. Special construction techniques have been used to overcome the swelling problem. Acid proof bricks have been used at temperatures as high as 589K (600°F). With proper construction techniques higher temperatures are possible.

The pertinent characteristics of available materials with known compatibility with sulfuric acid is summarized in Table 2. Precious metals meet all the prerequisites, however their very high cost for this application is prohibitive. High silicon containing alloys, such as Duriron have acceptable corrosion rates up to the boiling point under normal atmospheric pressures. Corrosion rates at higher pressures must be determined. Methods for joining the cast material to provide leak tight joints must be developed. Glass, because of its poor compatibility with superheated water, must be restricted to use at temperatures below 422K (300°F). Polymers are restricted because of their thermal instability at temperatures above 478K (400°F). Acid proof brick, because of its insulating properties, makes an excellent liner or barrier material for reducing temperatures between the process stream and the pressure vessel wall.

#### Materials For Use In The High Temperature - Superheated Steam Environment

In the reduction reactor, DR-1, the process stream which consists primarily of gaseous water and SO<sub>3</sub> is heated from 725 to 1144K (845 to 1600°F) and the SO<sub>3</sub> is reduced to SO<sub>2</sub> and O<sub>2</sub> by catalytic action. Compatibility data for structural materials exposed under these conditions are nonexistent. Some work however, has been done to investigate the behavior of a number of alloys in superheated steam at comparable temperatures. The most extensive research into the performance of materials in high temperature steam has been conducted by the ASME Research Committee on High Temperature Steam

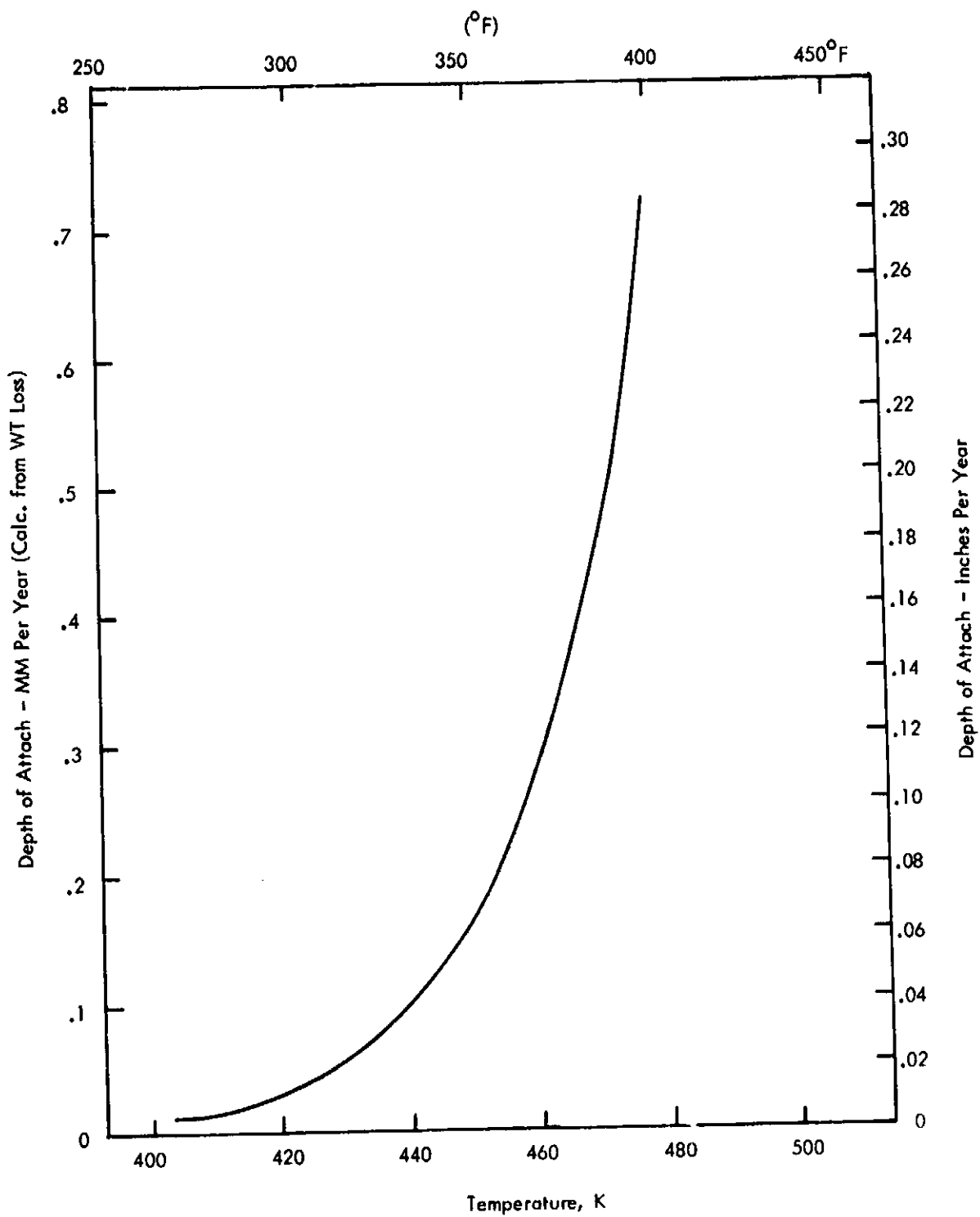


Figure 5. Affect of Superheated Water on Corrosion of Pyrex Glass (Corning No. 7740) (Reference 43)

TABLE 2

## SUMMARY OF CHARACTERISTICS OF AVAILABLE MATERIAL FOR USE IN SULFURIC ACID LOOP

Material	Compatibility With H <sub>2</sub> SO <sub>4</sub>	Compatibility With Superheated Water, SO <sub>3</sub> & SO <sub>2</sub>	Strength	Fabricability	Joinability	Thermal Conductivity	Relative Cost
Precious Metals (Gold, Platinum)	Excellent	Excellent	Fair	Must be used as clad on substrate	Good	Excellent	Very High
Metals High in Silicon (Duriron)	Excellent	Poor	Fair	Available as castings	Poor	Fair	Moderate
Glasses (Pyrex)	Excellent below 422K	Poor	Poor	Must be used on metal substrate	Poor	Poor	Low
Polymers (Teflon)	Excellent below 478K	Poor	Poor	Must be used on metal substrate	Good	Poor	Low
Acid Proof Bricks	Excellent	Excellent	Fair	Available as bricks and simple shapes	---	Poor	Low

Generation (Reference 44). Test results indicated that highly alloyed superalloys, such as Inconel 600, Incoloy 800, Hastelloy X, etc., promise a high degree of probability of meeting the requirements imposed by the operating conditions in DR-1. Alloys high in chromium which exhibit excellent oxidation resistance in air, also hold up well in superheated steam. The introduction of SO<sub>3</sub>, SO<sub>2</sub> and O<sub>2</sub> into the superheated steam introduce another degree of complexity. Thermodynamic analysis indicates that under the expected oxidizing conditions, sulfidation corrosion of nickel will not be a problem. Experimental data under DR-1 operating conditions will be required to verify material corrosion behavior.

#### Recommended Programs

- Because of the difficulties expected in determining the acceptability of materials for application in the system under the operating condition specified in Section 4.5, a revised set of operating conditions is being specified for the system conceptual design to be performed in Task III. These revisions include a reduction in pressure, and hence saturation temperature, of the sulfuric acid decomposition system and a change in the configuration of heat exchangers in the system. These revisions are discussed in Section 4.5.2.4.
- The corrosion behavior of Duriron, cast iron containing 15 percent silicon, in contact with boiling sulfuric acid over the concentration range of 80 to 100 percent under pressures up to 2069 kPa (300 psi) must be determined for an extended period of time, e.g., >10,000 hours.
- Investigate the sulfuric acid corrosion resistance of steel substrates coated with chemical-vapor-deposited silicon. Recent advances in coating technology have made it possible to produce complex geometrical shapes with a uniform adherent coatings. Steel which has been fabricated to a final shape can be siliconized by deposition of a layer of silicon of an appropriate thickness followed by a heat treatment to diffuse the silicon into the substrate. The resulting structure has a surface with a high silicon content which is highly resistant to sulfuric acid corrosion. The corrosion behavior of such a structure under boiling acid conditions must be determined.
- Ceramics such as silicon carbide, silicon nitride, and cermets (77 Cr-23 Al<sub>2</sub>O<sub>3</sub>) possess excellent resistance to sulfuric acid corrosion at ambient temperature and at low acid concentration. These materials have excellent thermal conductivity, can be fabricated into tubing of limited lengths, and can be joined by brazing. They possess sufficient potential to warrant further characterization.

APPENDIX B

TECHNOLOGY STATUS OF THE SULFUR CYCLE  
WATER DECOMPOSITION SYSTEM

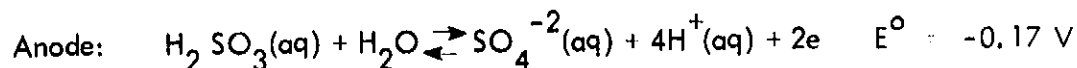
## TECHNOLOGY STATUS OF THE SULFUR CYCLE WATER DECOMPOSITION SYSTEM

### Electrochemical Hydrogen Generation

The Westinghouse Sulfur Cycle water-splitting process, based on the oxidation of  $\text{SO}_2$  to  $\text{SO}_3$  with subsequent thermal reduction of  $\text{SO}_3$ , requires that a means be found to carry out the following reactions:

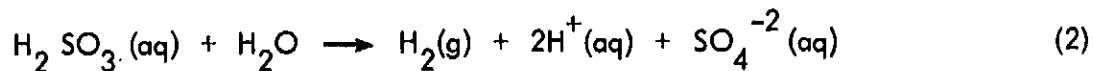


Although this reaction is not spontaneous and cannot be thermally driven, it may be accomplished electrochemically in an acid electrolyte by coupling the following half-cell reactions:



It should be noted that sulfur dioxide,  $\text{SO}_2$ , dissolves in an aqueous strong acid to yield sulfurous acid,  $\text{H}_2\text{SO}_3$ .

From the above, it may be concluded that, under standard conditions, the minimum driving voltage for the reaction



is 0.17 volts, which compares very favorably with the corresponding value of 1.23 volts for the electrolysis of water, i.e.,



Earlier work at Westinghouse confirmed that Reaction 2 proceeds substantially as written by operation of an electrolytic cell with platinized platinum electrodes in 50 w/o sulfuric acid at room temperature. However, with the anode and cathode compartments separated only by a sintered glass frit, the formation of a white solid simultaneous with the evolution of hydrogen was observed. This white powder was later identified as sulfur.

Examination of Table 1, which lists the standard reduction potentials of sulfur-containing species in acid solutions, reveals that sulfurous acid will depolarize the cathode reaction (see half-cell Reaction 2). If enough  $\text{H}_2\text{SO}_3$  is supplied to the cathode, no hydrogen will be evolved. Furthermore, sulfur formed by this reaction can also act as a cathode depolarizer, also inhibiting hydrogen evolution (see half-cell Reaction 4). Sulfur deposition is therefore to be expected if sulfurous acid is not excluded from the catholyte.

Juda and Moulton (Reference 45) did not report sulfur deposition when they used sulfur dioxide as an anodic depolarizer in an electrolysis cell operating at 368K in 30 w/o sulfuric acid. The important difference between their work and the preliminary Westinghouse work was that Juda and Moulton employed a flow-through electrode, i.e., the sulfurous acid solution was forced through a platinum-catalyzed porous carbon electrode under current, so that the solution was depleted of  $\text{H}_2\text{SO}_3$  by the time it reached the interelectrode electrolyte. Under these circumstances, sulfur deposition at the cathode could not occur.

Two other papers (References 46, 47) which discuss the electrocatalytic oxidation of sulfurous acid make no comment on the processes occurring at the cathodes of their systems. Das and Roy (Reference 46), who used an experimental apparatus similar to that used by Westinghouse, must have observed sulfur deposition but reported only on the anode polarizations. Wiesener (Reference 47) did similarly.

Sulfurous acid migration from the catholyte to the anolyte was fully inhibited by the simple and elegant experimental procedure devised by Bowman and Onstott (Reference 48). The use of a membrane and slight overpressuring of the catholyte resulted in the total avoidance of sulfur deposition at the cathode, and thus 100 percent current efficiency for hydrogen production.

In contrast to the complex situation existing at the cathode, only one reaction, i.e., the electro-oxidation of sulfurous acid, occurs at the anode. The extent to which sulfurous acid depolarizes the anode (oxygen-evolution electrode) in an electrolysis cell is shown in Figure 1, which is taken from the work of Juda and Moulton (Reference 45). The depolarized cell operates at 0.8 V below the voltages required for water electrolysis.

The effect of temperature on the polarization characteristics of platinized platinum electrodes in the anodic oxidation of sulfurous acid in about 25 percent  $\text{H}_2\text{SO}_4$  is shown in Figure 2. Das and Roy (Reference 46) employed a saturated calomel electrode (SCE) in their experimentation. Using a value of 0.263 V for the SCE versus the hydrogen electrode in normal sulfuric acid (Reference 49), an approximate scale for the electrode polarization versus the normal hydrogen electrode is provided for purposes of comparison. Increasing temperature results in a lowering of the electrode polarization - the effect amounting to 125 mV at  $100 \text{ mA cm}^{-2}$  on going from 303K to 353K ( $30^\circ\text{C}$  to  $80^\circ\text{C}$ ).

Wiesener's (Reference 47) data for 27 w/o  $\text{H}_2\text{SO}_4$  at 333K ( $60^\circ\text{C}$ ) are shown in Figure 3. The best performing electrode consisted of air-, steam-, or carbon dioxide-activated carbon, catalyzed by platinum and a mixed oxide,  $\text{V}_2\text{O}_5 \cdot 3\text{Al}_2\text{O}_3$ . An

TABLE 1  
STANDARD REDUCTION POTENTIALS OF SULFUR-CONTAINING  
SPECIES AT 298K IN ACID SOLUTION

	<u>Reaction</u>	<u>Potential, Volts</u>
1.	$S_2O_6^{-2} + 4H^+ + 2e \rightleftharpoons 2H_2SO_3$	0.57
2.	$H_2SO_3 + 4H^+ + 4e \rightleftharpoons S + 3H_2O$	0.45
3.	$SO_4^{-2} + 4H^+ + 2e \rightleftharpoons H_2SO_3 + H_2O$	0.17
4.	$S + 2H^+ + 2e \rightleftharpoons H_2S$	0.141
5.	$S_4O_6^{-2} + 2e \rightleftharpoons 2S_2O_3^{-2}$	0.09
6.	$2H^+ + 2e \rightleftharpoons H_2(g)$	0.00
7.	$2H_2SO_3 + H^+ + 2e \rightleftharpoons HS_2O_4^- + 2H_2O$	-0.08
8.	$2SO_4^{-2} + 4H^+ + 2e \rightleftharpoons S_2O_6^{-2} + H_2O$	-0.22



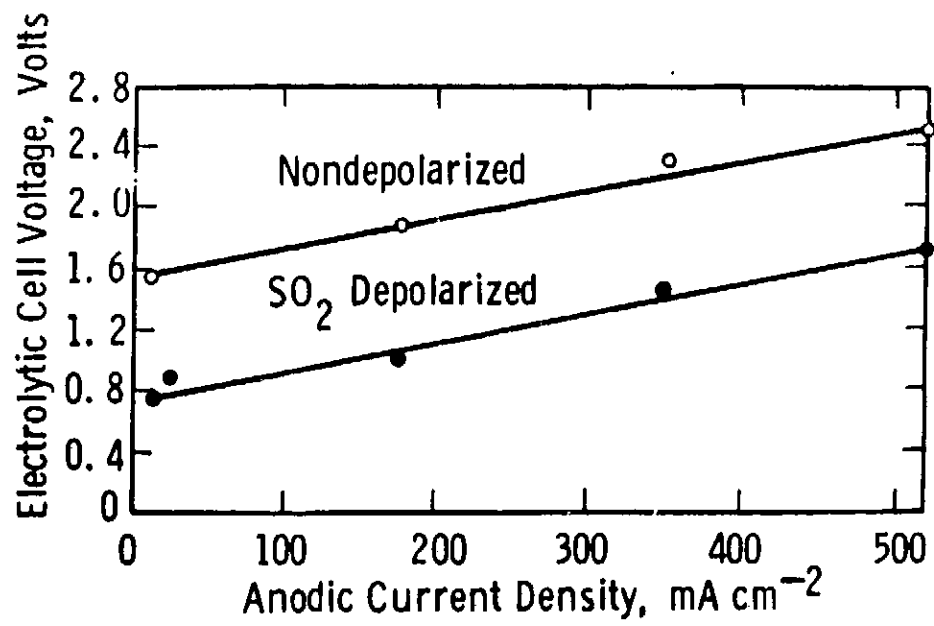


Figure 1. Effect of SO<sub>2</sub> on Electrolysis (After Juda and Moulton)

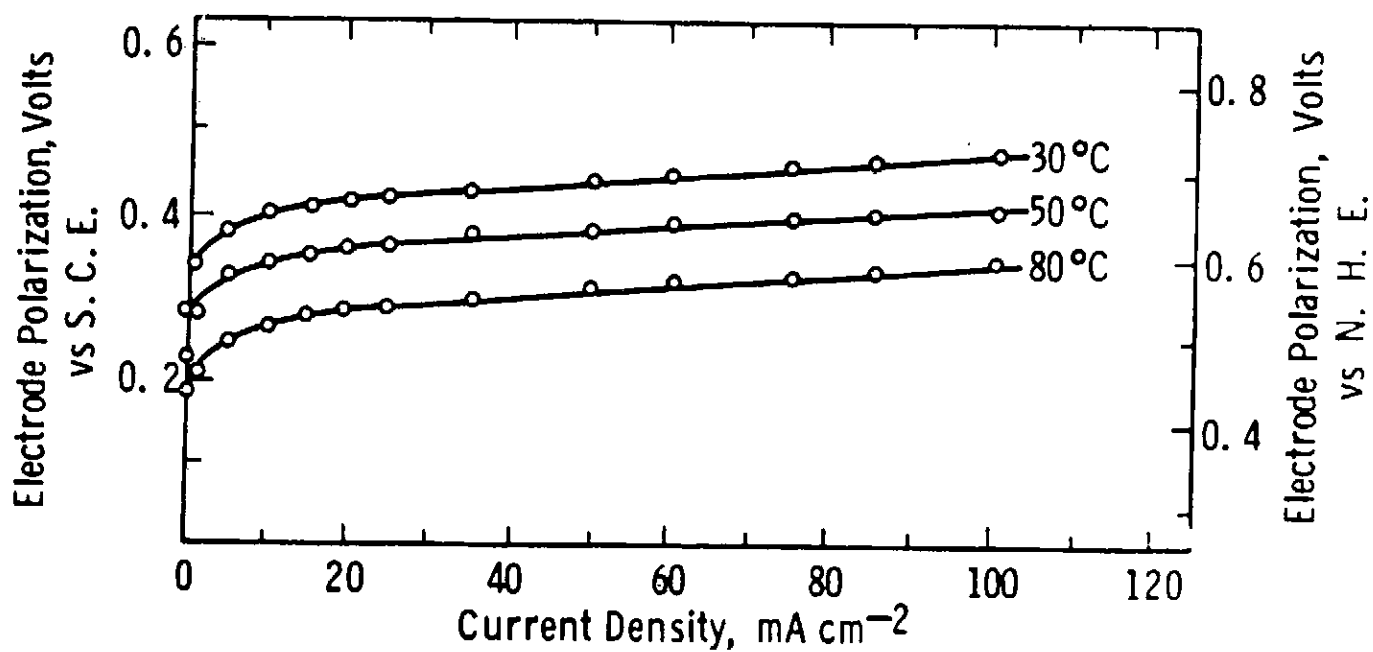


Figure 2. Polarization Characteristics of SO<sub>2</sub> Oxidation on Platinized Platinum Electrodes in 6N H<sub>2</sub>SO<sub>4</sub> at Different Temperatures (After Das and Roy)

approximate scale, to allow polarization values to be read in mV versus the normal hydrogen electrode, was constructed by the use of data (Reference 50) for the cell,  $H_2/H_2SO_4/Hg_2SO_4/Hg$ , at  $60^\circ C$ , and is included in Figure 3.

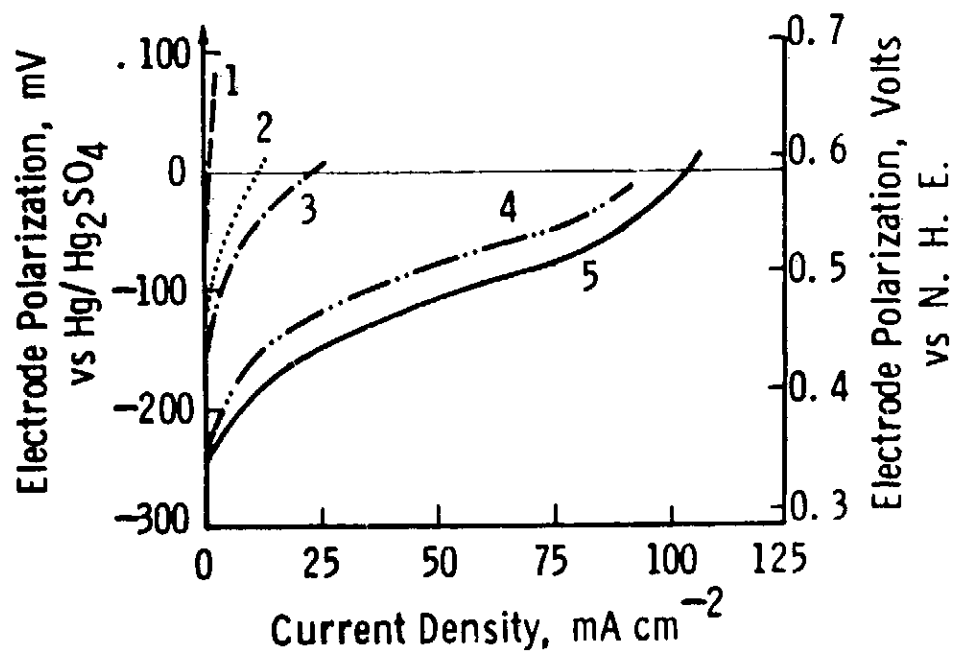
A summary of the relevant results of Das and Roy and Wiesener is presented in Table 2. Platinized platinum is not as effective an anodic electrocatalyst as platinum black. Wiesener's best performing electrode compares very favorably with the platinum black electrodes of Das and Roy. Electrolytic cell voltages of 0.7 V or less at  $100 \text{ mA cm}^{-2}$  should be achievable with this electrode, if the cell is operated at temperatures of  $333 \text{ K}$  ( $60^\circ C$ ) or greater with a platinized platinum hydrogen-evolution electrode ( $\eta \sim 0.07 \text{ V}$  at  $100 \text{ mA cm}^{-2}$ ) and an interelectrode spacing of 5 mm or less ( $\rho(H_2SO_4) \sim 1 \Omega \text{ cm}$  at  $333 \text{ K}$ ).

The results of Bowman and Onstott (Reference 48) for cells operating in  $SO_2$ -saturated  $2M H_2SO_4$  is shown in Figure 4. The pronounced effect of temperature on the cell voltage is obvious. The cell voltage at  $100 \text{ mA/cm}^2$  decreased from 900 mV to 750 mV when the temperature of operation is increased from  $295 \text{ K}$  ( $22^\circ C$ ) to  $353 \text{ K}$  ( $80^\circ C$ ). The data of Das and Roy (Reference 46), presented above, indicate that the voltage decrease is mainly due to a reduction of the activation polarization at the anode.

The main thrust of the experimental work funded and performed by Westinghouse to date has been to demonstrate technical feasibility, i.e., cell operation for extended periods with little or no sulfur deposition (current efficiencies in excess of 99 percent) and with acceptable voltage efficiencies at practical current densities (cell voltage  $< 0.6 \text{ V}$  at  $200 \text{ mA/cm}^2$ ). The suggestions of Bowman and Onstott (Reference 48) regarding the use of a membrane to separate the catholyte and anolyte, as well as catholyte overpressure, were incorporated into the experimental apparatus.

Figure 5 summarizes and puts into perspective the current density-voltage relationships observed in the Westinghouse work to date. The upper dotted line represents typical room temperature ( $22$  to  $30^\circ C$ ) observations of other investigators in  $17$ - $27 \text{ w/o } H_2SO_4$ , while the lower dotted line indicates the best of the high temperature data in other work. The two upper solid lines represent early data observed in  $50 \text{ w/o } H_2SO_4$  at  $303 \text{ K}$  ( $30^\circ C$ ) with the Westinghouse cell design. The break at approximately  $100 \text{ mA/cm}^2$  indicates the onset of a limiting current density phenomena due to the failure to maintain adequate activity of sulfuric acid at the anode. When due attention was paid to anode placement and the method of anolyte saturation with  $SO_2$ , the lowest solid line data set was observed at about  $303 \text{ K}$  ( $30^\circ C$ ) in  $50 \text{ w/o } H_2SO_4$ . With the assurance of an approximately  $150 \text{ mV}$  drop in cell voltage on raising the temperature to  $363 \text{ K}$  ( $90^\circ C$ ), cell voltages of  $< 0.65 \text{ V}$  at current densities of  $200 \text{ mA/cm}^2$  are seen to be achievable.

In summary, electrolytic cell operation, without sulfur deposition at the cathode and with about 100 percent current efficiency for hydrogen production has been successfully conducted over extended periods. Thus, the technical feasibility of  $SO_2$  depolarized electrolyzers has been demonstrated.



NOTE:

- 1 - Carbon
- 2 - Activated Carbon
- 3 - Activated Carbon +  $\text{V}_2\text{O}_5 \cdot 3\text{Al}_2\text{O}_3$
- 4 - Activated Carbon + Pt
- 5 - Activated Carbon + Pt +  $\text{V}_2\text{O}_5 \cdot 3\text{Al}_2\text{O}_3$

Figure 3. Effect of Activation and Catalysts on the Current Density-Potential Characteristics of a Carbon Electrode in the Oxidation of Sulfurous Acid - Temperature;  $60^\circ\text{C}$ : Electrolyte 27 w/o  $\text{H}_2\text{SO}_4$  (Reference 47)

TABLE 2

SUMMARY OF DATA OF WIESENER, AND DAS AND ROY,  
FOR THE ANODIC OXIDATION OF SULFUROUS ACID

Anode Material	H <sub>2</sub> SO <sub>4</sub> Conc. (w/o)	Temp. (K)	Polarization at 100 mA cm <sup>-2</sup> (mV vs. N. H. E.)	Reference
Platinum black	25	303	640	46
		323	585	46
		353	550	46
Platinized platinum	25	303	735	46
		323	670	46
		353	610	46
Gas-activated carbon - Pt catalyst	27	333	610	47
Carbon - Pt - 3 Al <sub>2</sub> O <sub>3</sub> · 2 O <sub>5</sub>	27	333	575	47

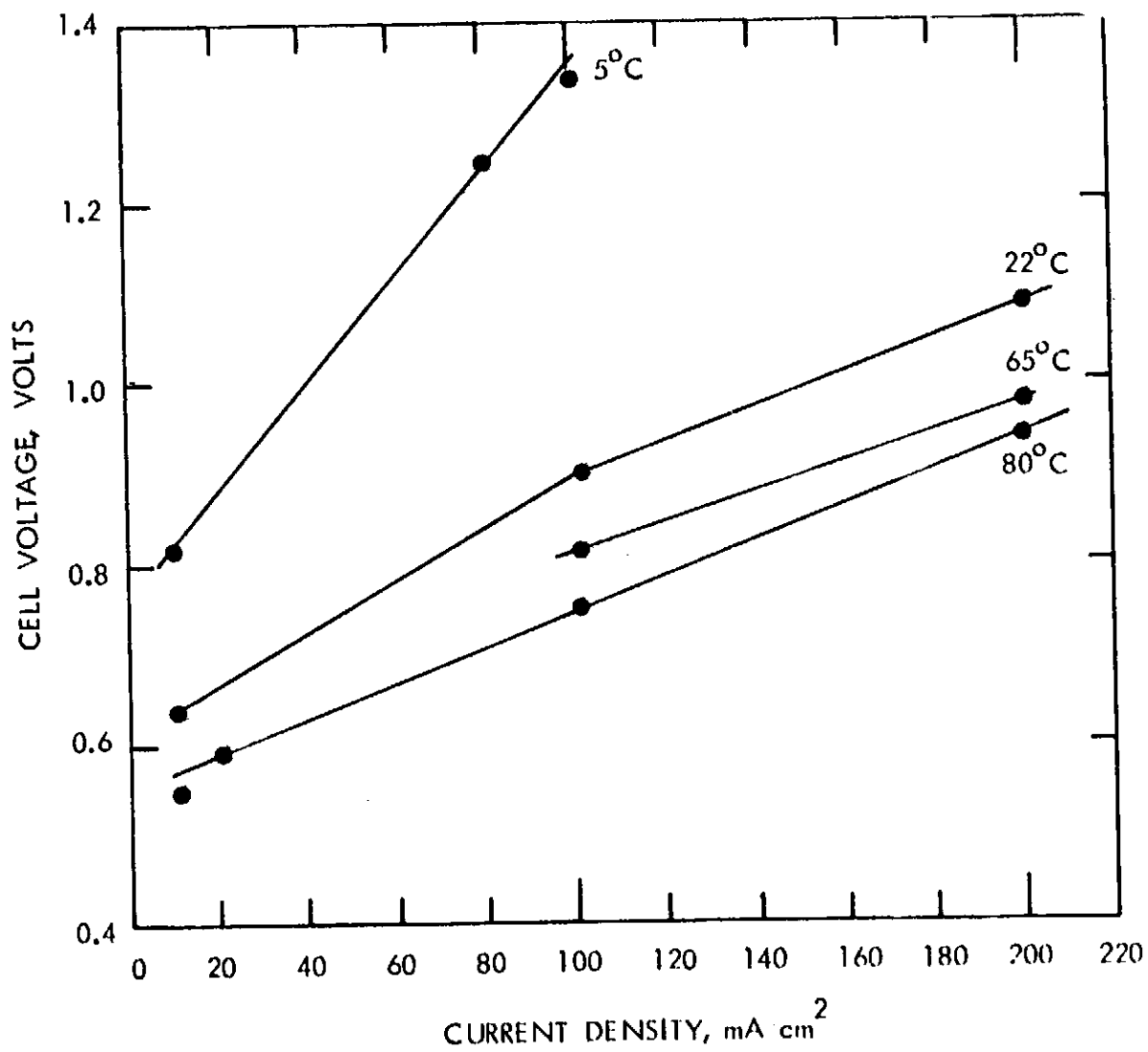


Figure 4. Electrolyzer Performance with Platinum Black Electrodes in 2M H<sub>2</sub> SO<sub>4</sub> Solutions at Different Temperatures (after Bowman and Onstott, IASL)

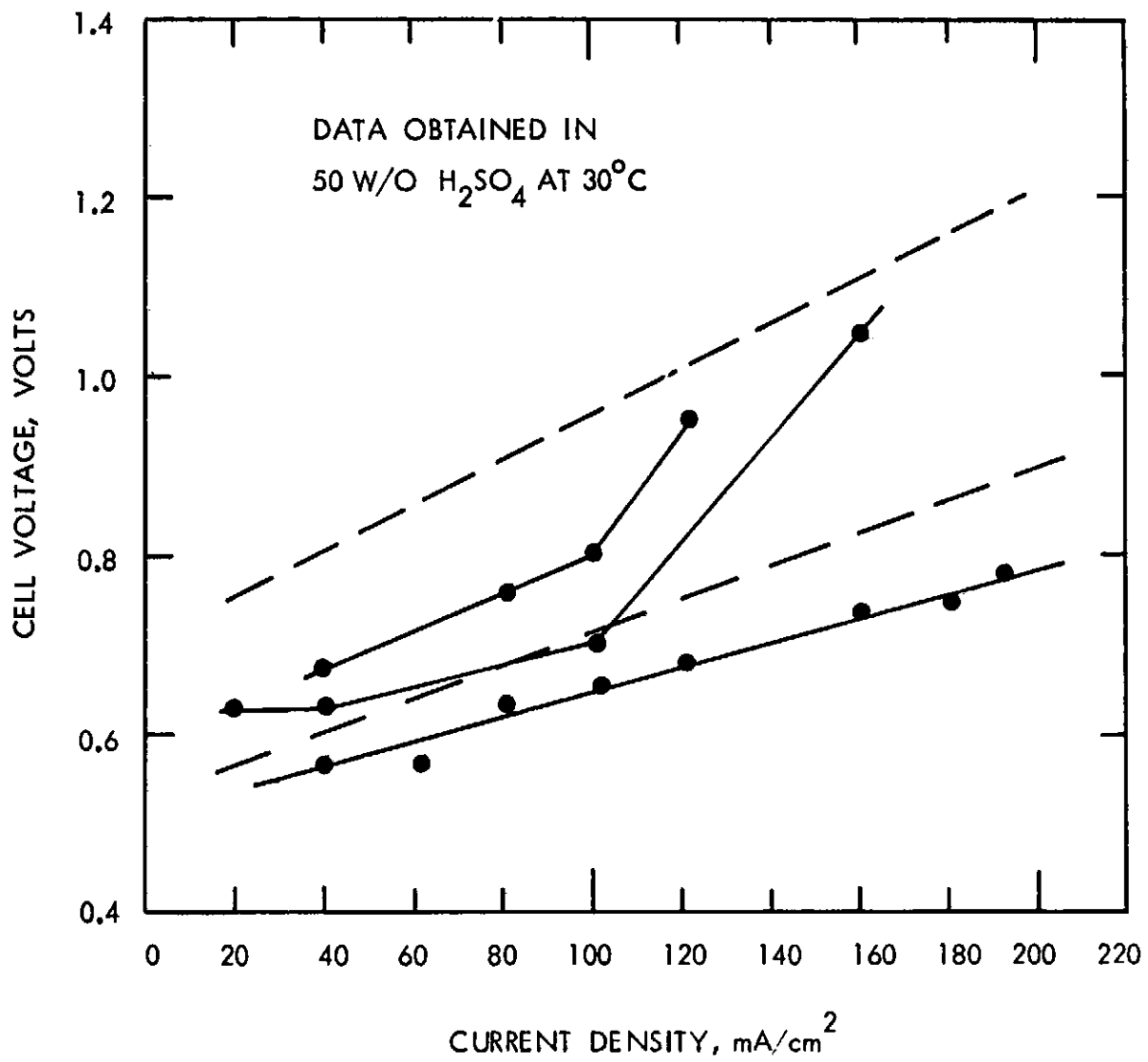


Figure 5. Recent Electrolyzer Performance Results

### Sulfur Trioxide Reduction

A substantial portion of the thermal energy entering the hydrogen generation process is introduced in the sulfur trioxide thermal reduction reactor. Consequently, the thermal reduction reactor is simultaneously a chemical reactor as well as a process heat exchanger. The design of such a piece of equipment is sensitive to both the heat and mass transfer characteristics of the system. The employment of large tubes and low overall temperature differences leads to a situation where the rate at which the endothermic chemical reaction proceeds is limited by the heat transfer rate. Similarly, the use of very small tubes and large temperature differences produces a design in which the mass transfer and chemical reaction rates, rather than the rate of heat transfer, influences the vessel size. Designing under heat transfer limited conditions leads to larger, more bulky equipment, whereas design under mass transfer limited conditions leads to poorer heat economy and more fragile equipment. The proper design involves an optimization with regard to both the heat and mass transfer characteristics of the system.

In order to define the range of gas residence time of technical interest, as well as to provide a basis for initiating design of the heat exchanger, preliminary concentration and axial temperature profiles along the exchanger/reactor were calculated for a near optimal design. These computations assumed a tube and shell exchanger using the same heat transfer coefficient calculated for the helium to helium intermediate heat exchanger in the nuclear heat source (VHTR) system. The chemical reaction was taken to be in equilibrium and the maximum allowable space velocity (or minimum residence time) consistent with equilibrium conversions at various temperatures was determined.

The design showed that for minimum catalyst activity, the catalyst must be capable of achieving equilibrium conversions along the entire length of the thermal reduction reactor at space velocities between 3500 and 6000  $\text{hr}^{-1}$  and at temperatures between 773 and 1173K (500 and 900°C). For more compact reactors, the catalyst must be capable of achieving equilibrium conversions by the time the process gas has reached the end of the reactor (temperatures about 1173K for space velocities between 30,000 and 60,000  $\text{hr}^{-1}$ ).

The purpose of the sulfur trioxide decomposition program is to identify a catalyst with sufficient activity and life for use in the  $\text{SO}_3$  thermal reduction reactor. Accordingly, Westinghouse constructed an experimental apparatus for investigating the kinetics of the thermal reduction of sulfur trioxide.

The first experiments run on this apparatus have been to determine the degree of reaction reversal to be expected upon quenching the high temperature gas mixture expected from the thermal reducer. This information is vital to an interpretation of the thermal reduction rate data taken later. Even more important, however, is the fact that if significant re-oxidation of  $\text{SO}_2$  would occur following the thermal reduction reactor, the entire process concept would be rendered either useless or highly inefficient.



The degree of reaction reversal to be expected was estimated by passing  $\text{SO}_2$  at a constant rate through the reactor with  $\text{N}_2$  and air carrier gases at various rates. Both hot and cold tests were performed. Under hot conditions, the mixture spent approximately two minutes flowing through the furnace ( $500 - 1000^\circ\text{C}$ ) and an additional two minutes in flowing from the  $500^\circ\text{C}$  furnace end to the analytical train. Under cold conditions, the gas mixtures traversed the system at room temperature. Residence times lower than four minutes were obtained by increasing the carrier flow while maintaining constant the  $\text{SO}_2$  rate.

A statistical analysis of the resultant data indicated identical  $\text{SO}_2$  rates into the analytic train for the  $\text{SO}_2/\text{N}_2$  hot runs and the  $\text{SO}_2/\text{air}$  cold runs. No effect upon residence time - up to four minutes - was observed in the  $\text{SO}_2/\text{air}$  hot runs. Additionally, the  $\text{SO}_2$  rate into the analytic train for the hot runs with air at all residence times was identical with that for the cold runs and the inert runs. Since over 100 determinations of  $\text{SO}_2$  rate were made during this period - none of which showed any significant statistical departure from the delivery rate - it is certain that  $\text{SO}_2$  reoxidation during quench will not be a problem so long as contact catalysts are not present.

The kinetics of two catalysts have also been investigated in the experimental apparatus. These catalysts, by reason of their proprietary nature, are designated as WX-1 and WX-2. For each catalyst, the reaction order was determined by testing integrated mass balance and reaction rate equations against the integral reactor data obtained in the system. Once the reaction order is known, the rate constant can be expressed as a function of a reaction group. This group contains a complex function of initial and final sulfur trioxide concentrations and varies with reaction order.

Plots of the reaction group versus  $1/T$  correspond to plotting the rate constant versus  $1/T$ . Figure 6 shows the curves obtained by plotting the data for catalyst WX-1. The agreement between predicted and experimental results is shown in Figure 7.

Figure 8 illustrates the expected conversions to be obtained with this catalyst at various temperatures and space velocities. The region of interest for the process heat exchanger is encompassed by space velocities between  $3000$  and  $8000 \text{ hr}^{-1}$ . As this clearly shows, WX-1 is a poor catalyst in this range at temperatures below  $1233\text{K}$  ( $950^\circ\text{C}$ ). Similarly, based upon the data to date there is no reason to expect it to be an effective catalyst below  $1073\text{K}$  ( $800^\circ\text{C}$ ), even at very low space velocities.

Data for the WX-2 catalyst is summarized in Figures 9 through 13. This catalyst was studied at space velocities of  $1000$ ,  $10,000$ ,  $30,000$ , and  $60,000 \text{ hr}^{-1}$ . Figure 9 plots the data obtained at  $60,000 \text{ hr}^{-1}$  according to the proposed rate equation. As predicted, the data yields a straight line. Figure 10, for  $30,000 \text{ hr}^{-1}$ , also shows a straight line which is parallel to the obtained at  $60,000 \text{ hr}^{-1}$ . The graphs at  $1000$  and  $10,000 \text{ hr}^{-1}$ , Figure 11, are different. Data plotted according to the model for these space velocities yield two superimposed curves. The fact that identical data was obtained at two different space velocities suggested that the

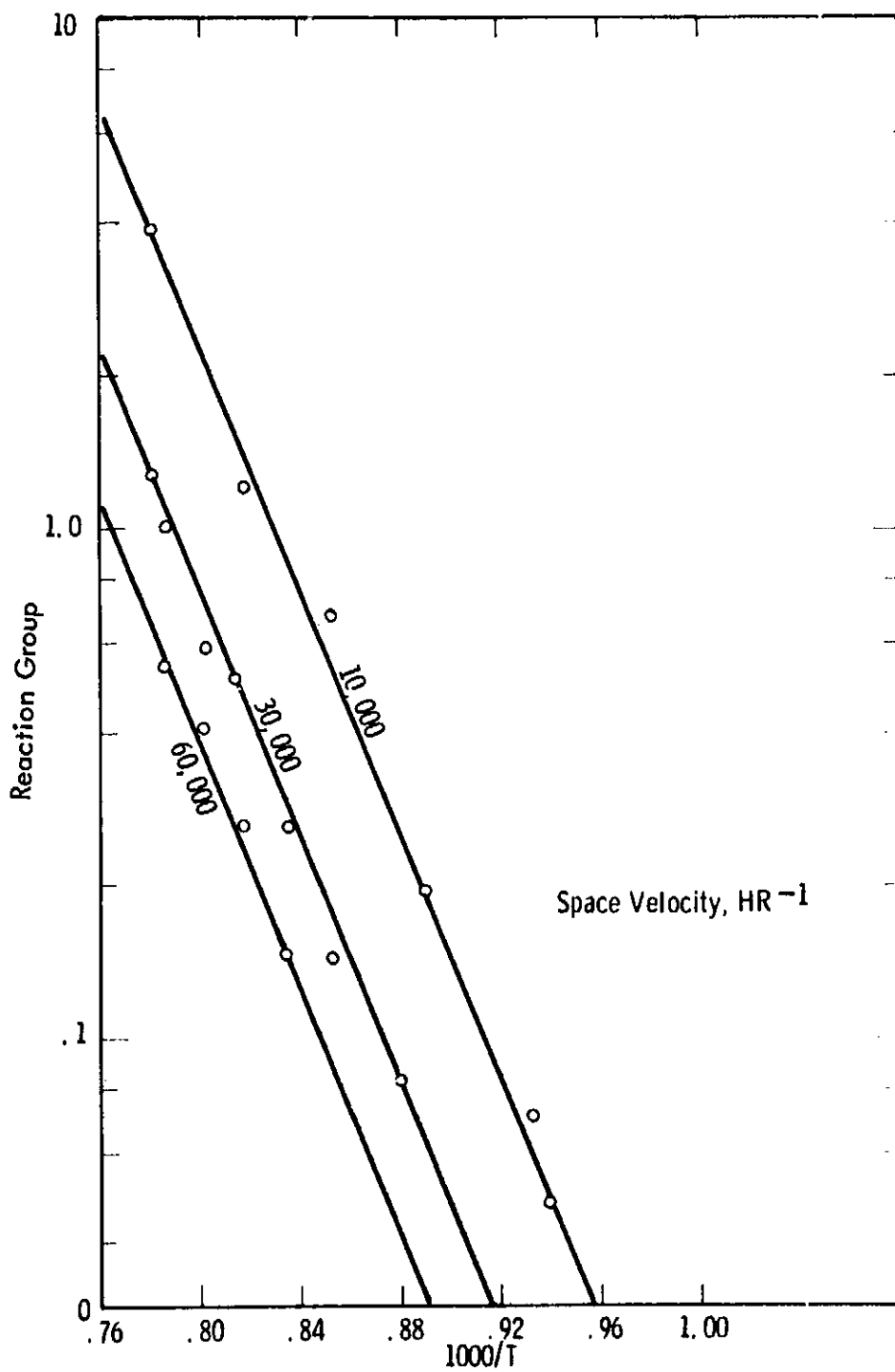


Figure 6. Arrhenius Plot of Sulfur Trioxide Reduction Data Obtained using WX-1 Catalyst

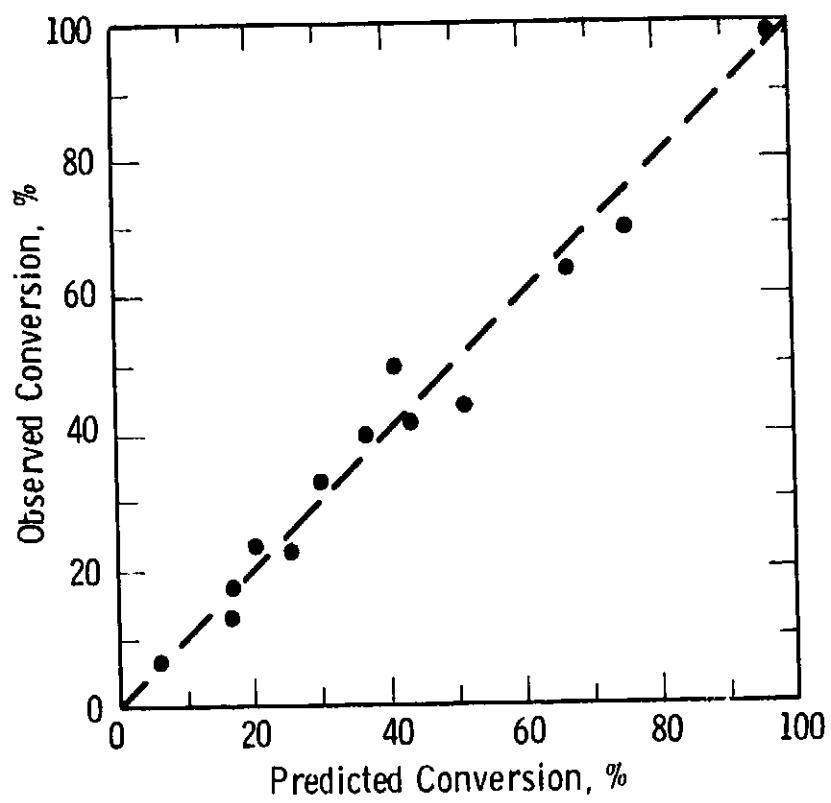


Figure 7. Agreement Between Observed Conversions and Those Predicted by Equation 5 for WX-1 Catalyst

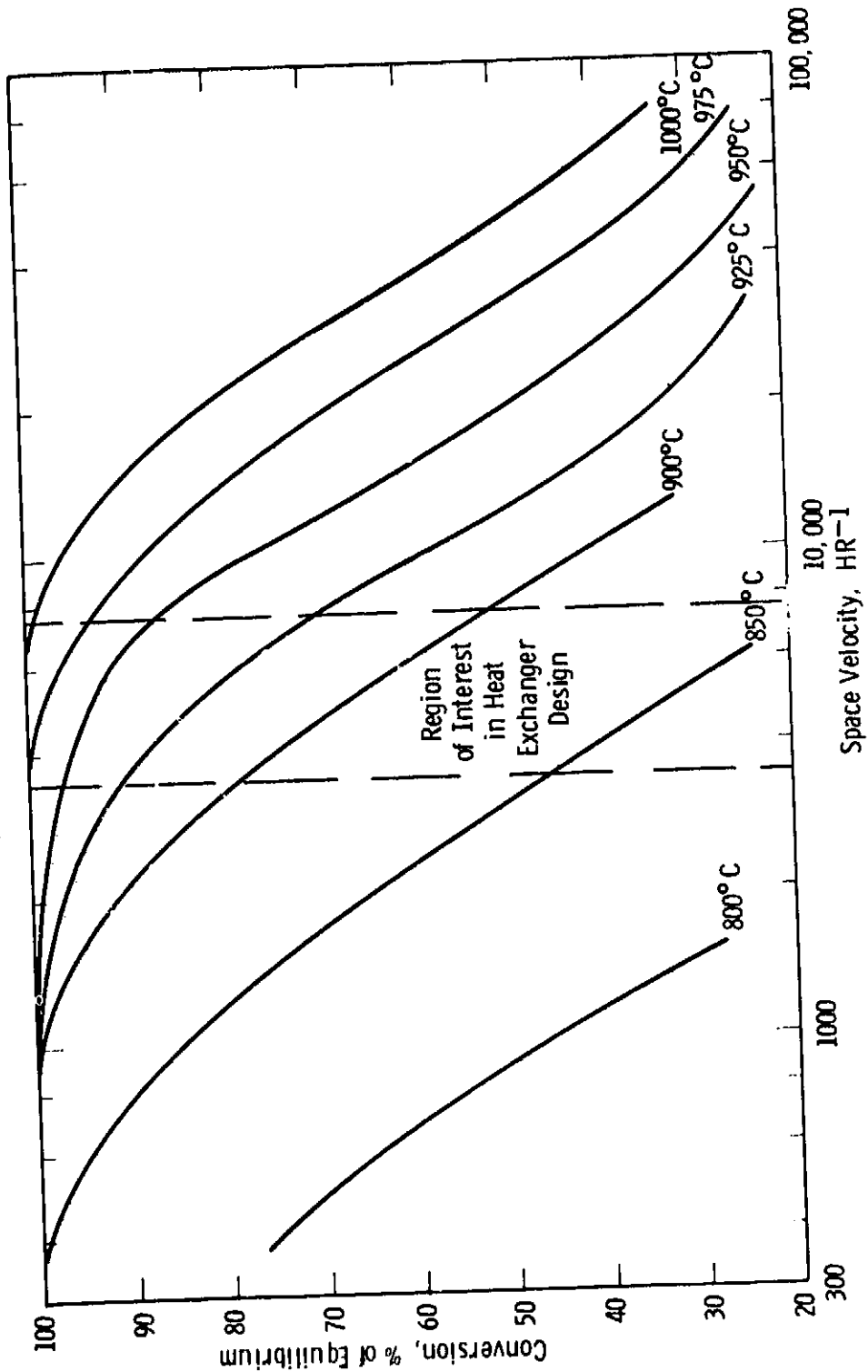


Figure 8. Predicted Sulfur Trioxide Conversions Over WX-1 Catalyst At Atmospheric Pressure

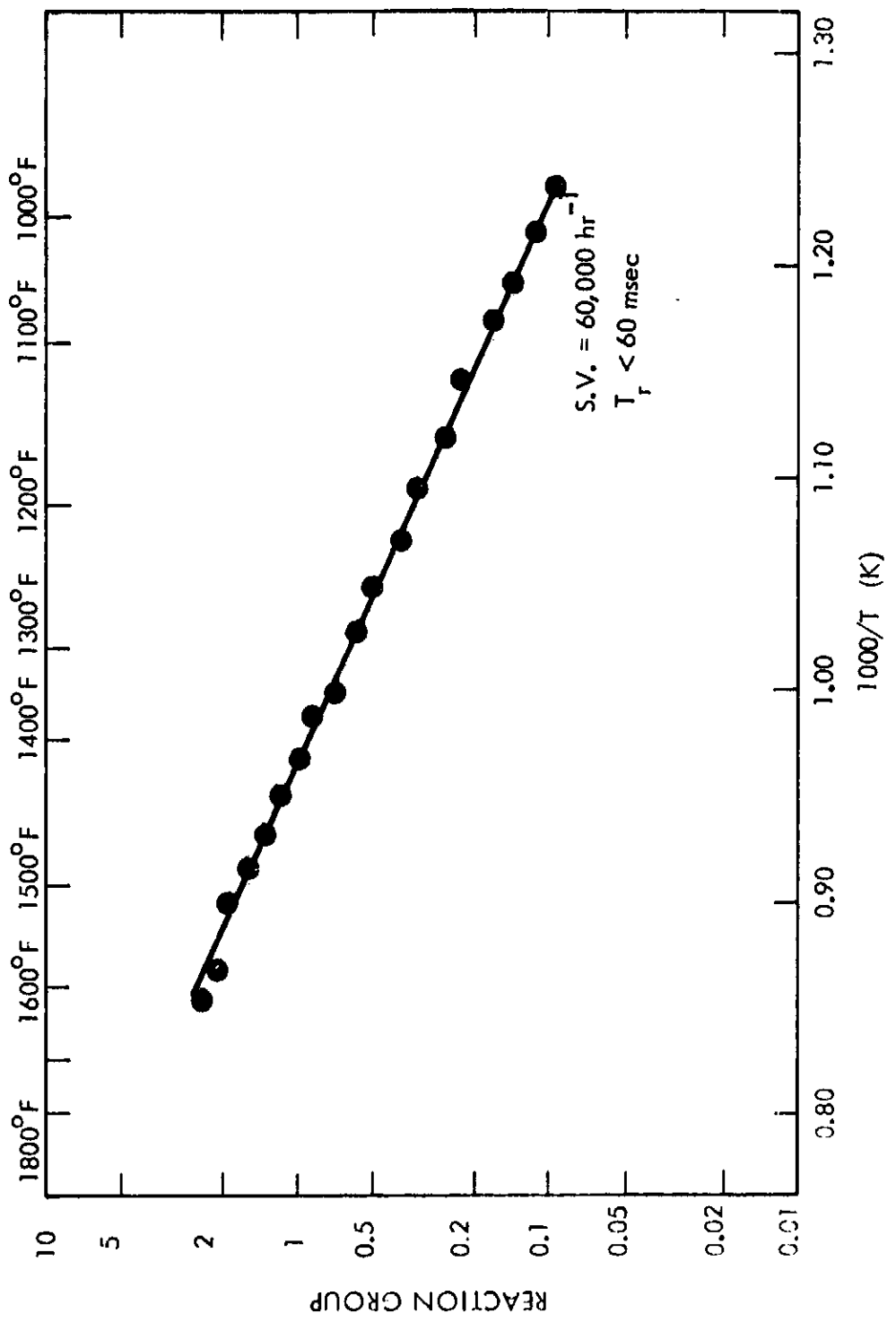


Figure 9. Sulfur Trioxide Thermal Reduction Reactor Catalyst Evaluation Results

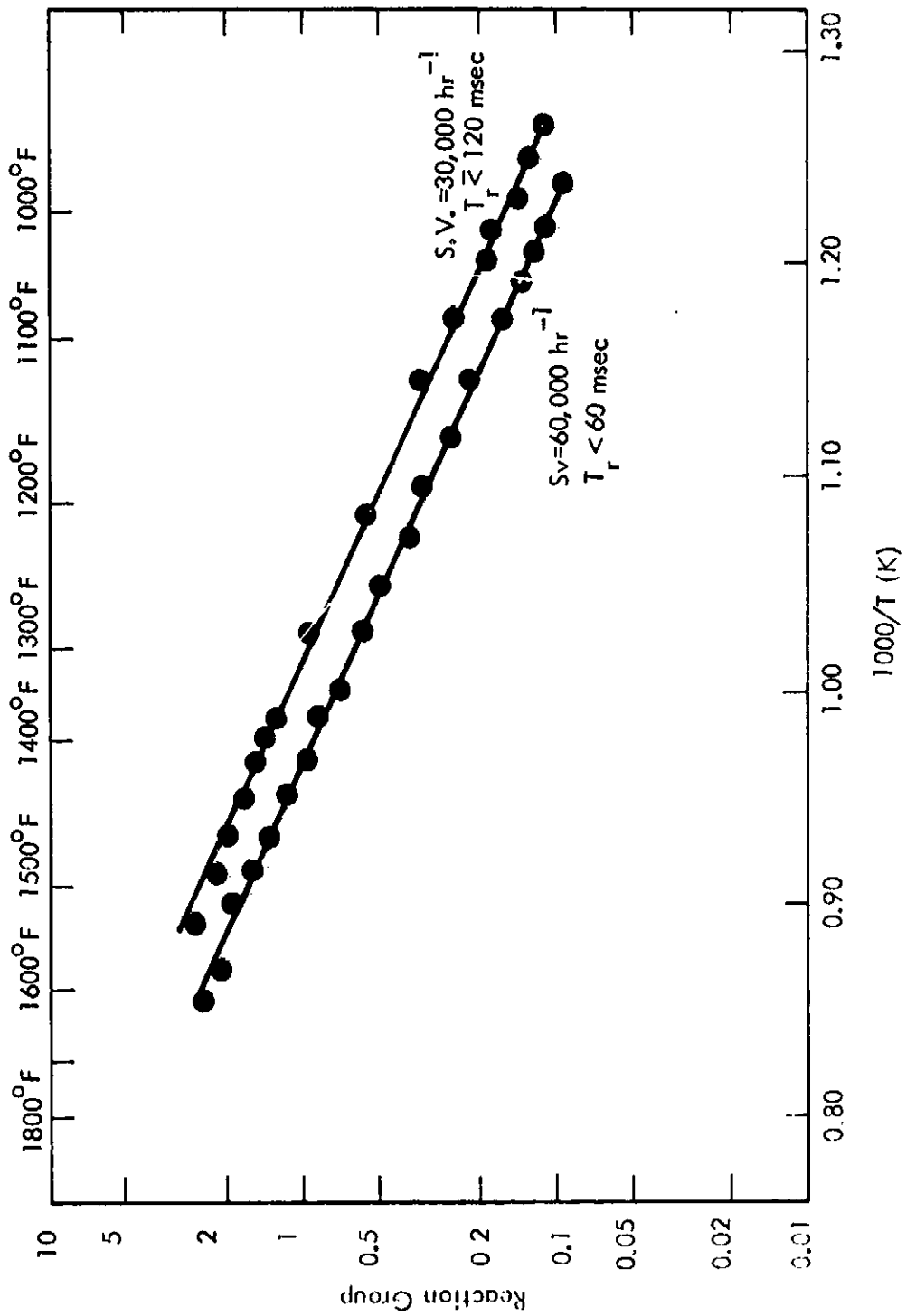


Figure 10. Sulfur Trioxide Thermal Reduction Reactor Catalyst Evaluation Results

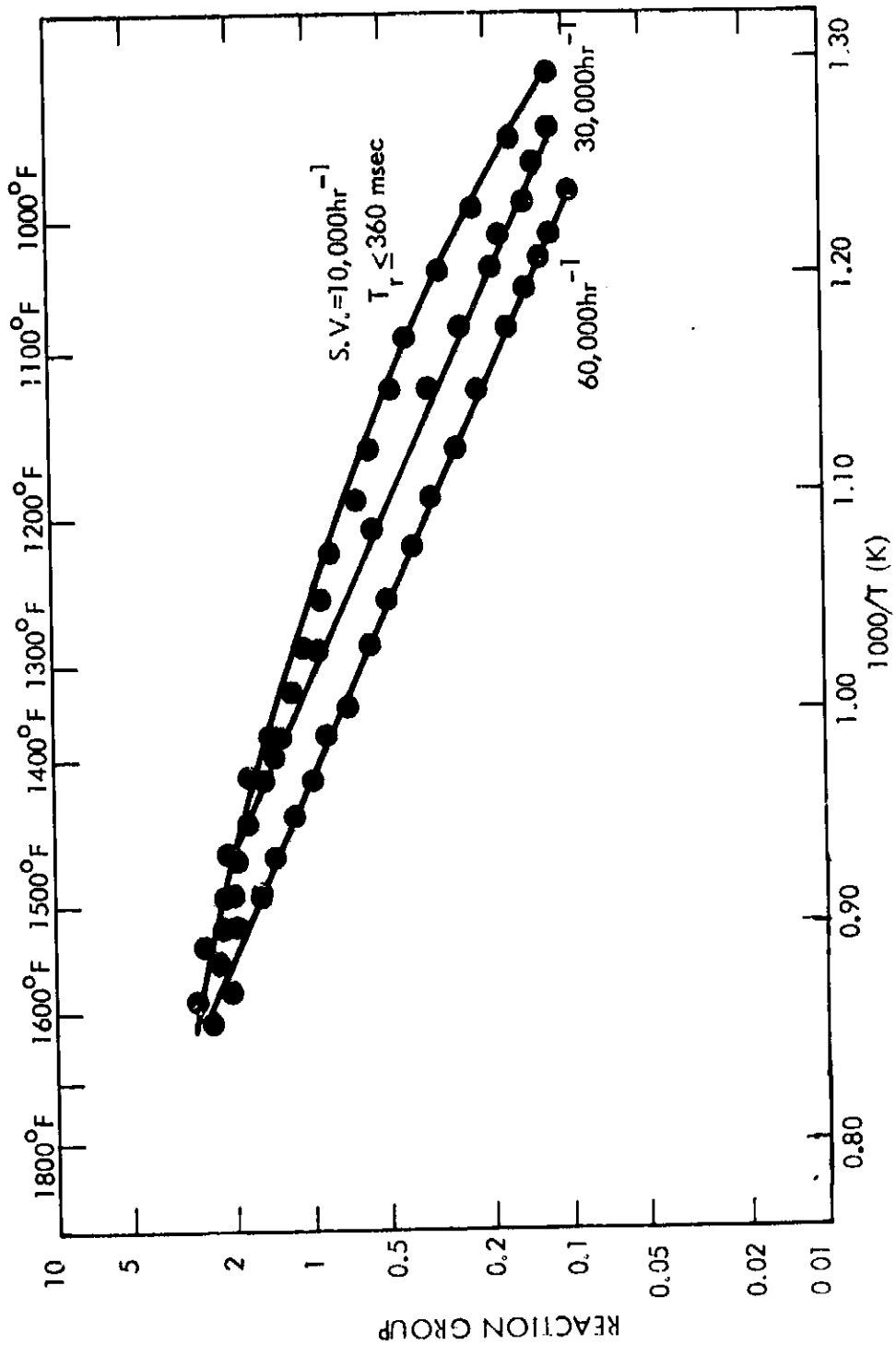


Figure 11. Sulfur Trioxide Thermal Reduction Reactor Catalyst Evaluation Results

reaction was at equilibrium over the entire temperature range of interest for the given space velocities. A calculated equilibrium curve superimposes over the curves in Figure 12, supporting this hypothesis. A 1000 hour life test was conducted using the WX-2 catalyst. As Figure 13 indicates, the catalyst maintained its initial activity throughout the life test.

The data from both catalysts support the kinetic model. So far, only the WX-2 catalyst shows sufficient activity and life for use in the  $\text{SO}_3$  thermal reduction reactor. Accordingly, these catalyst results are being employed in the reactor design being conducted in Task III.



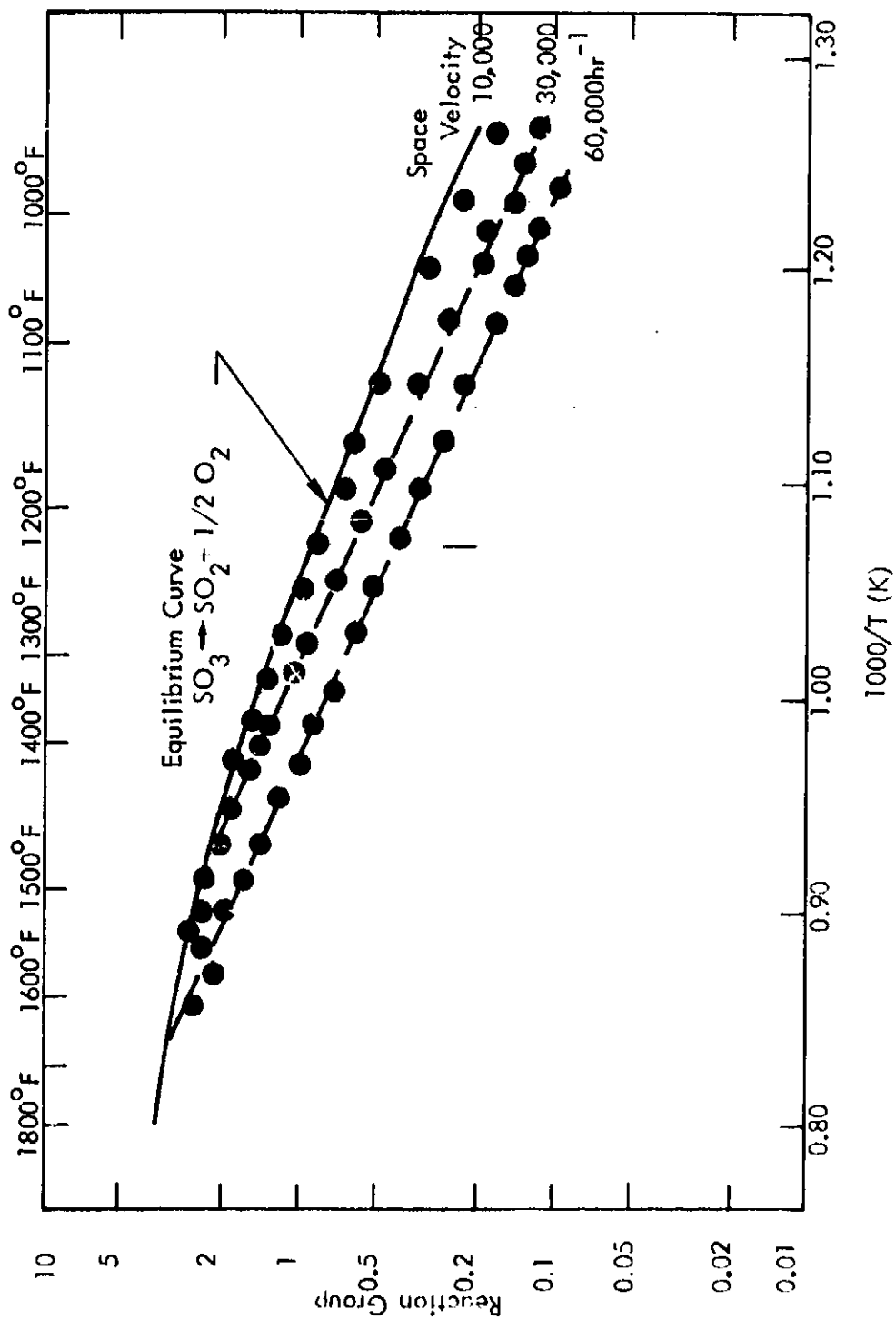


Figure 12. Sulfur Trioxide Thermal Reduction Reactor Catalyst Evaluation Results

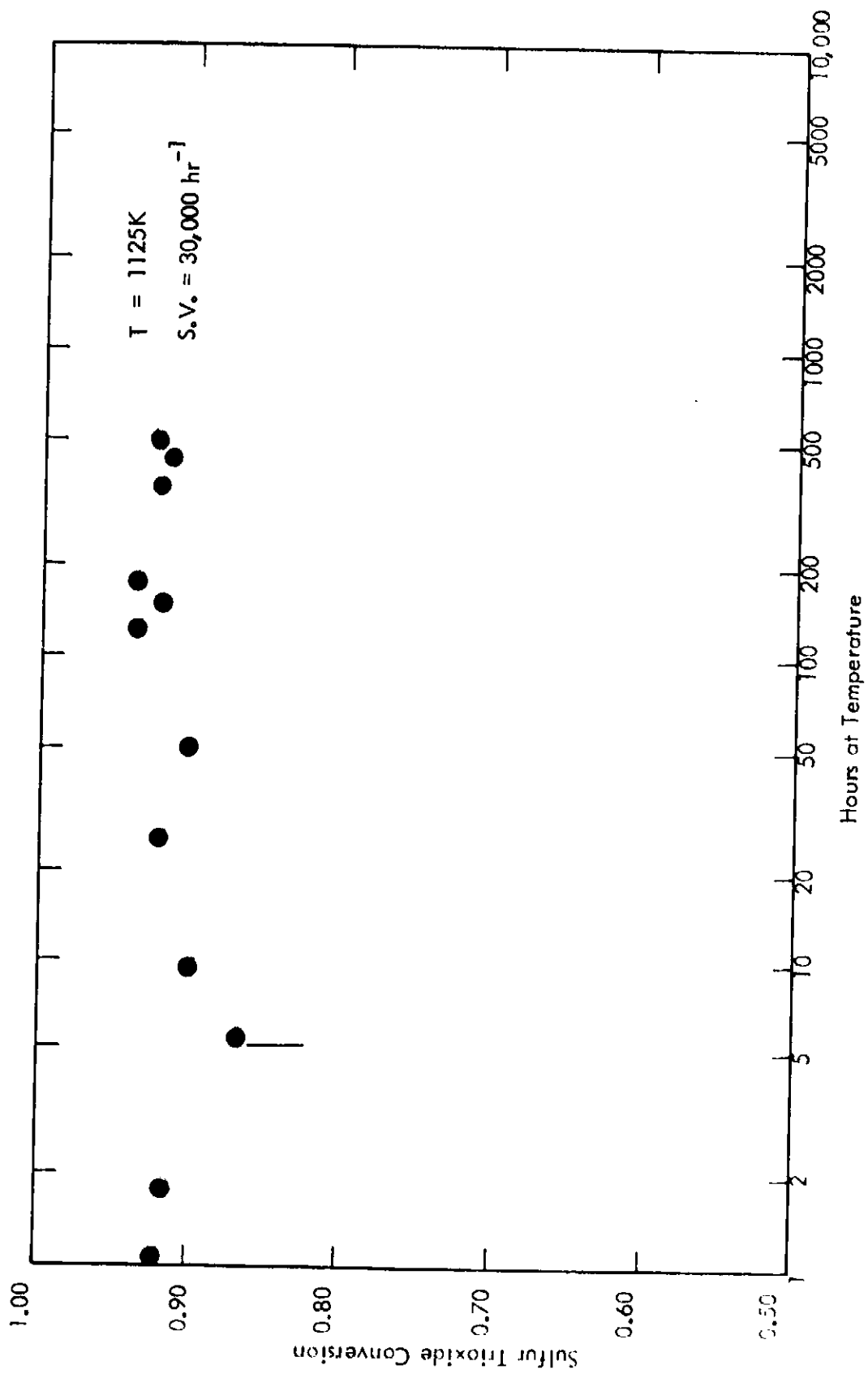


Figure 13. Sulfur Trioxide Thermal Reduction Reactor Catalyst Life Test Results

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