COMPUTER-AIDED ANALYSIS OF CRITICAL TECHNOLOGIES FOR HYDROGEN MANUFACTURE

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PREFACE

This informal working paper documents the results of a study to demonstrate and assess the applicability of flowsheet simulation or a screening tool to aid in process research planning. Very crude models were used for three processes for hydrogen manufacture. Because of limitations in the model the process and economic results presented herein should be used only as an illustration of qualitative trends. We have not checked the data on which these results are based and make no claim for the exact numerical values.

The study demonstrated, however, that rigorous flowsheet simulation using ASPEN PLUS with preliminary process economics is an excellent tool for evaluation processes at the research stage. If more time and data were available, the models could be readily upgraded to give realistic quantitative comparisons.

ABSTRACT

The development of new chemical processes is often hampered by exhaustive research into many variations in several alternative production methods. There is a real need for a tool which can provide early information to help guide the selection of the most promising routes and identify the critical areas of research to make the final process most efficient. This study uses the example of hydrogen manufacture, considered very important for the future of synfuels technology, to demonstrate how computer flowsheet simulation can fill this need.

Three different hydrogen production processes were modeled with the ASPEN flowsheet simulation system. Steam reforming and partial oxidation of methane were studied separately and then compared. For each model the process efficiency, defined in terms of product purity, yield, and cost, was analyzed as a function of the operating conditions. Trends in behavior were plotted and methodologies for process optimization found. On comparing the processes, steam reforming was identified as the more cost effective process. Partial oxidation, although resulting in lower initial capital investment for the same size plant, has higher operating costs associated with the need for a pure oxygen feed. This process is competitive with steam reforming only if a very low cost source of oxygen is available.

The third process simulated was electrolysis of water. This demonstrated the method by which flowsheet simulation can be used to compare processes based on very different technologies. It was found that because of the cost of the large amount of electricity needed, electrolysis produces hydrogen at several times the cost as that of the steam reforming process. In addition, the capital expenditure for a large scale electrolysis plant is much higher than the same size steam reforming facility because of the high cost of the necessary electrolysis equipment. This suggests that electrolysis is not a viable alternative for hydrogen manufacture on the scale needed for future synfuels processes.

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INTRODUCTION

Although it is the third most abundant element by atom, hydrogen does not appear naturally anywhere on earth in its pure form. Generating hydrogen therefore requires the chemical decomposition of a heavier material containing hydrogen, followed by the separation of the gaseous hydrogen from other side-products. (9) Because hydrogen has been a very important feed stock in the chemical and petrochemical industries and because the production of it is typically quite expensive, a great deal of work and money has gone into the development and optimization of the processes used to generate hydrogen. In the future hydrogen should become an even more important raw material, for although there is a world oil surplus at this time, the certainty of long-term limited resources suggests the eventual need for large quantities of hydrogen either as a fuel or in synthetic gas production. (4)

The oil crisis in the mid 1970´s focused the world´s attention on the problem of limited resources and the need to find alternative ways to insure reliable and inexpensive energy sources for the future. (9) One of the critical areas identified was the need for efficient, cheap, high-volume hydrogen production. As a result, an explosion of research ensued on many fronts. People from private industry, universities, and the United States government all began large scale research projects. Some looked at production methods involving partial oxidation of hydrocarbons (e.g. 1, 2, 4, and 11). Others looked at improving the now favored process: steam reforming of hydrocarbons (e.g. 1, 4, 7, 11, and 13). Some looked for ways to make the simplest method, direct electrolysis of water, cost competitive despite the inherent thermodynamic inefficiency of electricity generation and the high capital cost of high-volume electrolytic cells (e.g. 3, 4, and 5). Finally, some explored revolutionary production methods, including the once highly promising thermochemical cycles involving complex multi-reaction systems in which water is broken into its elements through the use of recycled reaction materials. (e.g. 4)

Among the many advancements forwarded by this volume of work has been one fact inherent to hydrogen production: there is a vast number of production and separation method combinations and no efficient way to compare and choose among them. Some studies involved detailed design and cost calculations for different processes (4), but the inflexibility of this "brute-force" method becomes clear when one faces the task of repeating all of these calculations when a break-through is made in, for example, the physical reliability of very high temperature reactors. Another comparative approach has been the use of detailed computer models to predict operating conditions and ultimate process costs (11). Here again an inherent inflexibility exists in that every time the process is modified in some way, a new computer program for the new process must be generated.

In the hydrogen industry, then, there is a clear need for a tool to aid in the study and selection of alternative process pathways. An efficient method must be developed by which processes which are vastly different in concept and stage of development can be compared on an equal footing. With this tool, early development work could be guided so as to eliminate improbable processes and point out directions of greatest need for viable, low-cost production methods. The desire for such a comparative tool is not exclusive to hydrogen production: there is a general need in the whole chemical industry for an efficient methodology for process comparison.

This study focuses on one answer to this need: computer flowsheet simulation. With flowsheet simulation, the user is given a list of unit operations from which he may select. By taking those unit operations which are in the chemical process under study and connecting them appropriately with material flow streams, a flowsheet simulation is quickly developed. The user then has an efficient means of studying the effects of any relevant process inputs on any results of interest. The flexibility of this method over "brute-force" calculations and dedicated computer programs is clear when one considers the ease with which the unit operations can be moved around, inserted, or replaced in order to more fully explore process alternatives.

The goal of this study is to demonstrate the power of flowsheet simulation in studying, comparing, and optimizing alternative processes. Various means of hydrogen production, including steam reforming of methane, partial oxidation of methane, and electrolysis of water, have been selected for this demonstration because of the real and immediate need for this tool in this field as described above. The flowsheet simulator ASPENPLUS, developed at M.I.T. and now licensed by Aspen Technology, Inc., Cambridge, MA, was used for this work. This simulator has all of the unit operations necessary for simulating these hydrogen processes and has a comprehensive costing package with which capital and operating expenses can be easily calculated.

It should be noted that while every effort has been made to use realistic operating and cost numbers in these simulations, the emphasis of this work is on the methodology of flowsheet simulation and not the specific operating and cost conclusions found for hydrogen production. It is hoped that this demonstration will show the flexibility and applicability of flowsheet simulation to the study of alternative processes, and that engineers will use simulation in conjunction with actual data from existing or experimental facilities to make intelligent choices for the future.

I. PROCESS DESCRIPTIONS

STEAM REFORMING OF METHANE

The first process to be simulated was the current favored method for hydrogen production: steam reforming. There are many variations on this process, including a variety of ways of treating the synthesis gas produced in the reformer and of separating the pure hydrogen from the side products. Figure 1 shows a typical configuration, chosen because it is not overly complex and yet represents the average process in use today.

The heart of this production method is the reformer furnace at the top of the flowsheet. Two feeds enter this unit operation: steam and methane. Other hydrocarbons can be used as the hydrogen source, but methane was selected because of its common use and because of its high hydrogen to carbon ratio. After the feeds enter the reformer, they heat up and reaction takes place over a catalyst inside. The top of Figure 2 shows the reactions occuring in the reformer. Methane and water react to form hydrogen and carbon monoxide. The carbon monoxide can then react with water to produce more hydrogen and carbon dioxide. The overall reaction is highly endothermic, so the reformer furnace must supply heat to force the reactions to go

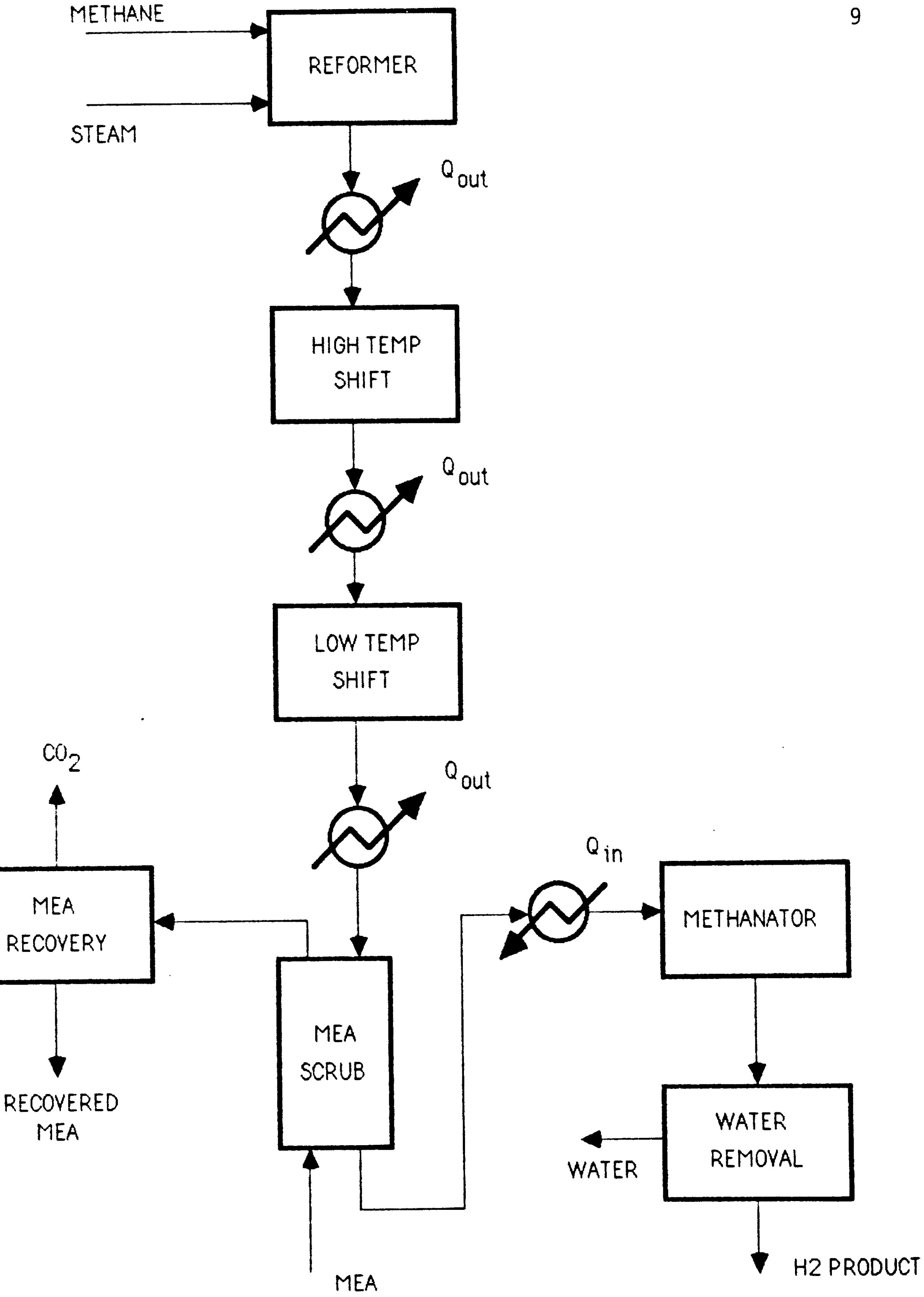


FIGURE 1: Process Flowsheet for Steam Reforming of Methane

- REFORMER REACTOR:

$$CH_4 + H_2O \longleftrightarrow 3\ H_2 + CO$$

$$CO + H_2O \longleftrightarrow CO_2 + H_2$$

Temperature = 900 - 1250 K
Pressure = 10 - 50 ATM
Steam: CH_4 = 3.0 - 5.0

- SHIFT REACTORS:

$$CO + H_2O \longleftrightarrow CO_2 + H_2$$

Temperature = 600 - 750 K (HIGH), 450 - 600K (LOW)
Pressure = < 80 ATM

- METHANATOR:

$$CO_2 + 4\,H_2 \longleftrightarrow CH_4 + 2\,H_2O$$

Temperature = 600 K

FIGURE 2: Chemical Reactions for Reactors in Steam Reforming Process

toward completion.

Also indicated on Figure 2 are broad ranges for the reformer conditions. The temperature range is limited by the effective range of the catalyst, and the pressure range is in part controlled by the need for high pressure hydrogen at the end of the process (i.e. keep the pressure high throughout the process to avoid the costs of compression at the end). The steam to methane ratio into the reformer is generally about 4:1. The excess steam helps drive both reactions toward the right, favoring greater hydrogen production, and also helps prevent carbon formation on the catalyst inside the reformer. (1)

The next step in the process, as shown in Figure 1, is a series of cooling and shift reaction steps. The reformer exit gases are cooled and sent to a high temperature shift reactor. Here some carbon monoxide is converted to hydrogen over a catalyst via the water gas shift reaction. The center section of Figure 2 shows the reaction involved. The exit from this reactor is cooled again and sent to a low temperature shift reactor where most of the remaining carbon monoxide is converted to carbon dioxide and hydrogen. Also shown in Figure 2 are ranges in operating conditions for the two temperature shift reactors. The temperatures are again limited by the catalyst constraints.

This two step shift process is favored because of the reaction equilibrium and cost of catalyst versus the process temperature. Low temperatures favor near complete conversion of carbon monoxide, but the catalysts active at low temperature tend to be more expensive to use. (11) The high temperature catalysts are cheaper, making it more cost effective to shift some of the carbon monoxide over these catalysts and use a low temperature catalyst only as a final, clean-up step.

The stream leaving the low temperature shift reactor should contain a large fraction of hydrogen, some carbon monoxide, some methane, and a small amount of carbon monoxide on a dry basis. The next step, as shown in Figure 1, is to remove the impurity carbon dioxide from the product stream. Many methods are in use, but for this simulation absorption with monoethanolamine (MEA) has been used. Here the gaseous product stream is contacted on a multi-stage basis with the amine. Essentially all of the carbon dioxide is removed in this way. The exit amine, heavy with carbon dioxide, is sent on for recovery and ultimate recycle. Usually, recovery is handled easily by simply heating the MEA and driving off the carbon dioxide. (4)

The product stream, now stripped of carbon dioxide, contains hydrogen, methane, and carbon monoxide on a dry basis. This stream is heated up so that the small amount of carbon monoxide which was not shifted in the shift reactors can be reacted in a methanator to produce the final product. The bottom of Figure 2 shows the reaction taking place in the catalytic methanator. A small amount of hydrogen is sacrificed to react with the carbon monoxide to give methane and water. As shown in Figure 1, all of the water in the product stream from the methanator is removed, and the final product, consisting only of hydrogen and methane, emerges.

PARTIAL OXIDATION OF METHANE

Another method for hydrogen production, which has essentially been replaced by steam reforming, is partial oxidation. This process was selected as the second to be simulated, for it is similar to steam reforming, providing an easy basis of comparison, and it was hoped that the simulation would demonstrate why steam reforming is favored. Figure 3 shows the partial oxidation flowsheet used. The only major difference between this flowsheet and the steam reforming one shown in Figure 1 is the oxidizer at the top. Because both processes generate a synthesis gas after their primary reactor, the exact same recovery process was used downstream.

The feed to the oxidizer consists of methane, oxygen, and steam. Here too, other hydrocarbons can be used, including coal, as the hydrogen source. Methane was selected simply to provide for easy comparison with the steam reforming results. The top of Figure 4 shows the desired reactions taking place inside the oxidizer. The oxygen is used to oxidize the methane to produce hydrogen and carbon monoxide. The steam reacts with the carbon

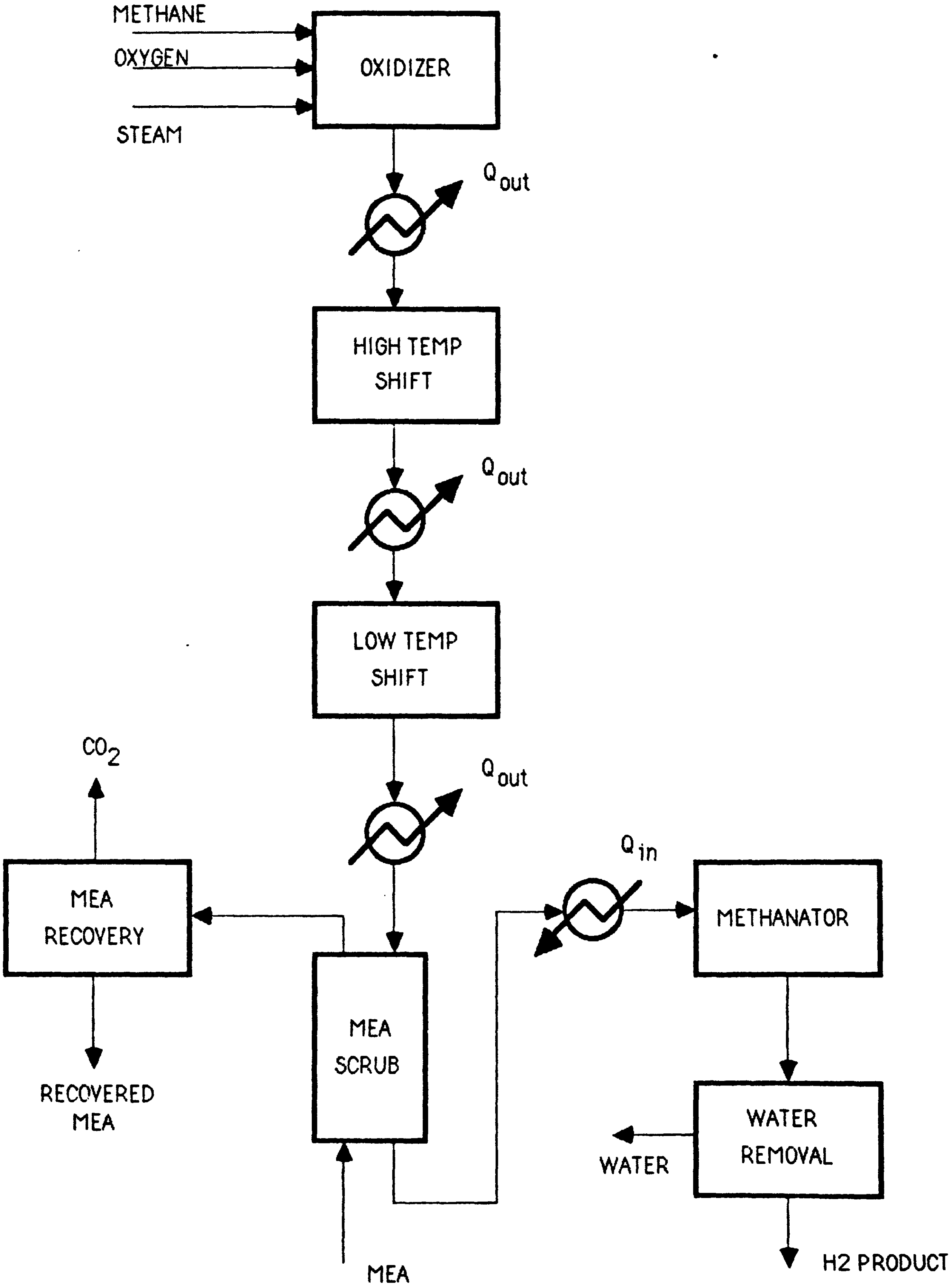


FIGURE 3: Process Flowsheet for Partial Oxidation of Methane

- OXIDATION REACTOR:

$$CH_4 + (1/2)\,O_2 \longleftrightarrow 2\,H_2 + CO$$

$$CO + H_2O \longleftrightarrow CO_2 + H_2$$

Temperature = 1050 - 1300 K
Pressure = 1 - 30 ATM
Steam: CH_4 = 0.5 - 1.5
O_2: CH_4 = 0.5 - 1.5

- SHIFT REACTORS:

$$CO + H_2O \longleftrightarrow CO_2 + H_2$$

Temperature = 600 - 750 K
Pressure = < 80 ATM

- METHANATOR:

$$CO_2 + 4\,H_2 \longleftrightarrow CH_4 + 2\,H_2O$$

Temperature = 600 K

FIGURE 4: Chemical Reactions for Reactors in Partial Oxidation Process

monoxide to produce more hydrogen and carbon dioxide.

Figure 4 also shows some ranges in operating conditions. Depending on these process conditions, the overall reaction may be either exothermic or endothermic. This points up the real advantage to the partial oxidation process: unlike steam reforming, little heat input is required in this primary reactor, providing for savings on capital to build the reactor and fuel costs while operating. The disadvantage is the need for relatively pure oxygen in large quantities. This usually requires building an on-site oxygen plant as well, making the oxygen an expensive feed stock. (11)

The steam to methane ratio for the oxidizer is far less than that in the reformer because water is not needed in the primary reaction. Generally a ratio of around 1.0 provides the necessary water to drive the second reaction toward the right. The oxygen to methane ratio is also generally near 1.0. It must be high enough to allow the first reaction to take place but cannot be so high as to allow full oxidation to take place, burning off the desired hydrogen.

The remainder of the partial oxidation flowsheet, as indicated in Figures 3 and 4, is the exact same as that for the steam reforming process.

ELECTROLYSIS OF WATER

The final hydrogen generation process simulated with this study was direct electrolysis of water. It is well known that electrical current, when applied to water in an electrolysis cell, causes water to split into gaseous hydrogen and oxygen. This process is by far the simplest way to generate hydrogen and has the advantage of producing almost 100% pure product with a minimum of separation equipment. It suffers, however, from the high cost associated with the large amount of electricity used and the large capital costs required for electrolysis cells necessary for high volume production. Electrolysis was selected for study so as to compare to the catalytic methods of reforming and oxidation with the completely different approach of electrolysis. It was hoped that the simulation would demonstrate the advantages and disadvantages between these processes, allowing for an intelligent selection of the appropriate process for future development.

Figure 5 shows the simple flowsheet involved with electrolysis. The water is fed to a cell where electricity is used to split it into its elements. The the product streams, oxygen and hydrogen, are then taken off. The pure oxygen created can be a bonus, however the high cost of liquifaction needed to economically ship oxygen any great distance negates this advantage unless the oxygen can be used on site. (4)

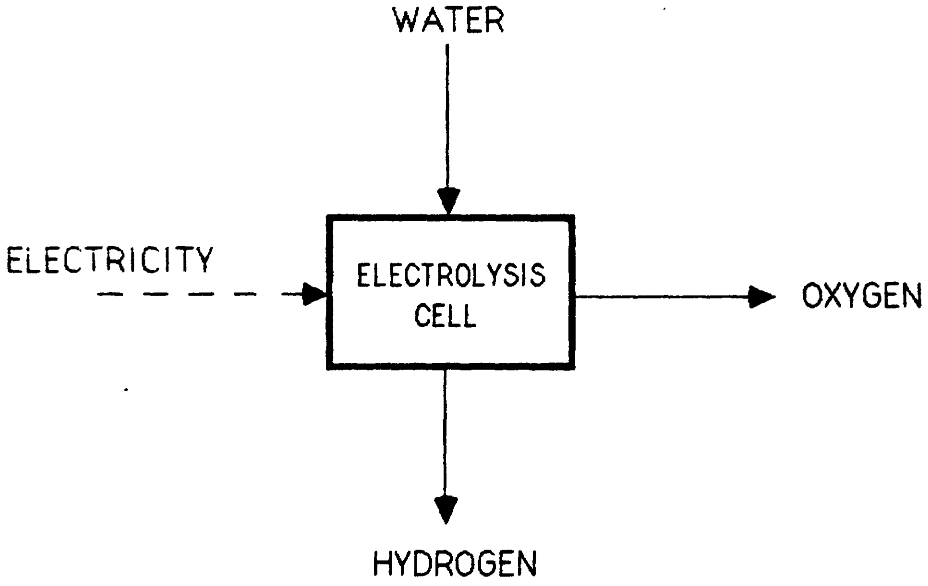


FIGURE 5: Process Flowsheet for Electrolysis of Water

- ELECTROLYSIS CELL:

$$H_2O + \text{electricity} \longleftrightarrow H_2 + (1/2)\,O_2$$

FIGURE 6: Reaction in Electolysis Process

Figure 6 shows what is happening chemically inside the electrolysis cell. Again, the simple nature of the process makes it attractive. The major complexity is involved with the electrolyte which is used inside the cell. Some systems use liquid electrolytes such as solutions of potassium hydroxide. In order to improve cell efficiency (theoretical power required divided by actual power used), some work was been done to develop newer electrolytes such as solid polymers. (4) For this simulation, it has been assumed that all of the feed water is converted to hydrogen and oxygen and that the overall cell efficiency is 85%.

II. ASPENPLUS FLOWSHEET SIMULATION

STEAM REFORMING OF METHANE

All of the simulations in this study were done with the ASPENPLUS flowsheet simulation system. For each process, the flowsheet was divided into its individual unit operations. For each unit operation, ASPENPLUS has a corresponding model or "block." Those blocks appearing in a given flowsheet are selected and connected by material flow streams. The operating conditions for the unit operations are entered and the feed streams are specified. The simulation can then be executed, and the desired results accessed. In addition, ASPENPLUS has a comprehensive costing section which allows the individual process units to be costed, leading to a calculation of the total capital investment. The costing section also calculates utility and raw material usage, labor, overhead, and depreciation so that a total operating cost can be reported.

Figure 7 shows the ASPEN block diagram for the steam reforming process. This shows all of the ASPEN blocks used in this simulation and the types of models they represent. Listing 1 in the appendix shows the actual ASPEN input language for this process. Comparison of

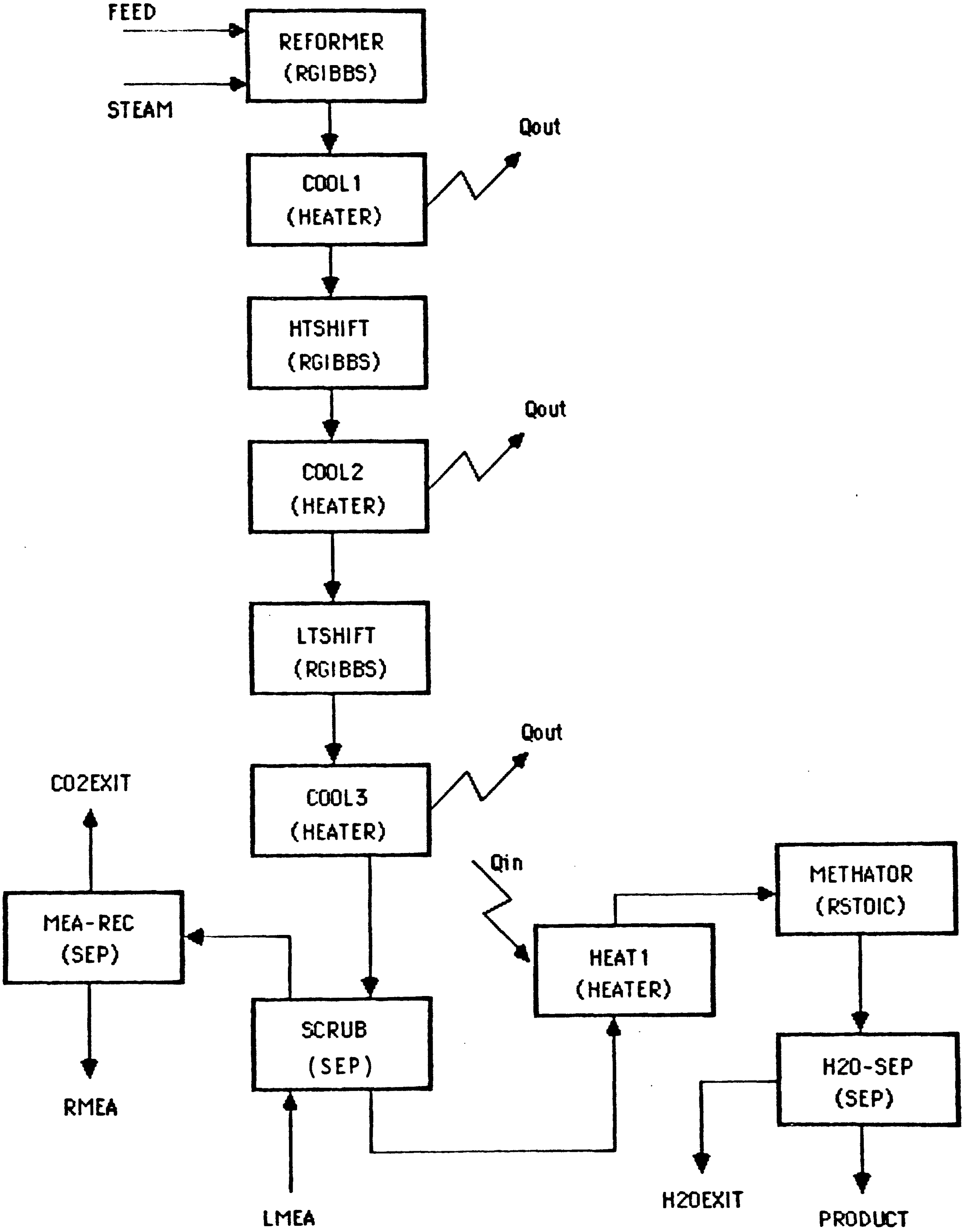


FIGURE 7: ASPEN block diagram for the Steam Reforming Process

Figure 7 with Figure 1 shows that the translation of flowsheet to ASPEN block diagram consisted of matching each step in the process with the appropriate ASPEN model.

The main reformer reactor is modeled with the ASPEN reactor block "RGIBBS." This is a model which uses Gibbs free energy to find the final equilibrium composition of the product stream. The components which are present - methane, water, hydrogen, carbon monoxide, and carbon dioxide - are entered in this block as are the operating conditions in the reformer. Optionally, the temperature approach to equilibrium can be entered to simulate incomplete reaction. For this simulation, the temperature approach to equilibrium for the methane reaction was set at -15 C. (8)

All of the heaters and coolers are modeled with "HEATER" blocks. These take as input the desired exit temperature and pressure and calculate the necessary heat duty based on the inlet stream conditions. This heat duty is then accessed by the costing section to determine heat exchanger and utility needs for the heating or cooling step.

Both the high temperature and low temperature shift reactors are also modeled with "RGIBBS" blocks. Again the species present and operating conditions are entered. For both blocks a temperature approach to equilibrium of +10 C was used for the shift reaction. (8)

It was assumed that 100% of the carbon dioxide is removed by the monoethanolamine (MEA) in the scrubber. For this reason, this step was modeled simply as a "SEP" block. This block takes the incoming flow of the gaseous product and MEA and directs the individual species present to the outlet streams with given separation fractions. For this simulation 100% of the MEA exits with the stream going to the MEA recovery unit as does 100% of the carbon dioxide. This stream goes to another "SEP" block, "MEA-REC" which removes the carbon dioxide and returns the recovered MEA. The remaining gaseous materials in the scrubber all exit to the heater and on to the methanator.

The methanator is the only reactor which is not modeled with "RGIBBS." It was assumed that all remaining carbon monoxide reacts to form water and methane (i.e. the reaction goes to completion). For this reason, the ASPEN reactor model "RSTOIC" was used. This model takes as input the stoichiometry of the reaction occurring and the conversion rate of that reaction. Here, a conversion rate of 1.0 was used.

The last unit in the flowsheet removes any water to produce a pure, dry product stream. This is a "SEP" block in which all of the water is directed to the water exit stream and all of the hydrogen and methane is taken off as product.

The costing section of the simulation accesses the important variables from around the flowsheet to calculate capital and operating costs. The heat duties are used to size units such as the reformer furnace, the cooling steps, and the heating step, and the utility rates, in terms of steam and fuel oil are calculated. Raw material usage, such as methane purchase cost, is also found. As will be discussed in the results section, one of the key uses for the costing section of the simulation was to take the production rate and operating cost and determine the production cost per million BTU of hydrogen for various operating conditions.

PARTIAL OXIDATION OF METHANE

Because of the similarity between the processes, the ASPEN simulation for partial oxidation was built directly on that already developed for steam reforming. Figure 8 shows the ASPEN block diagram for the partial oxidation process. Listing 2 in the Appendix is the corresponding ASPEN input language. The only real difference is in the first block - as mentioned above, the downstream processing of the synthesis gas is identical. For this process the oxidizer is modeled as a "RGIBBS" reactor. Instead of just methane and steam, though, an additional feed of pure oxygen is used. In the block, the presence of oxygen is added to the list of species found in the steam reformer reactor. It was assumed for this simulation that the reactions taking place go to equilibrium before exiting.

The remaining ASPEN blocks, input language, and operating conditions are the same as those discussed above

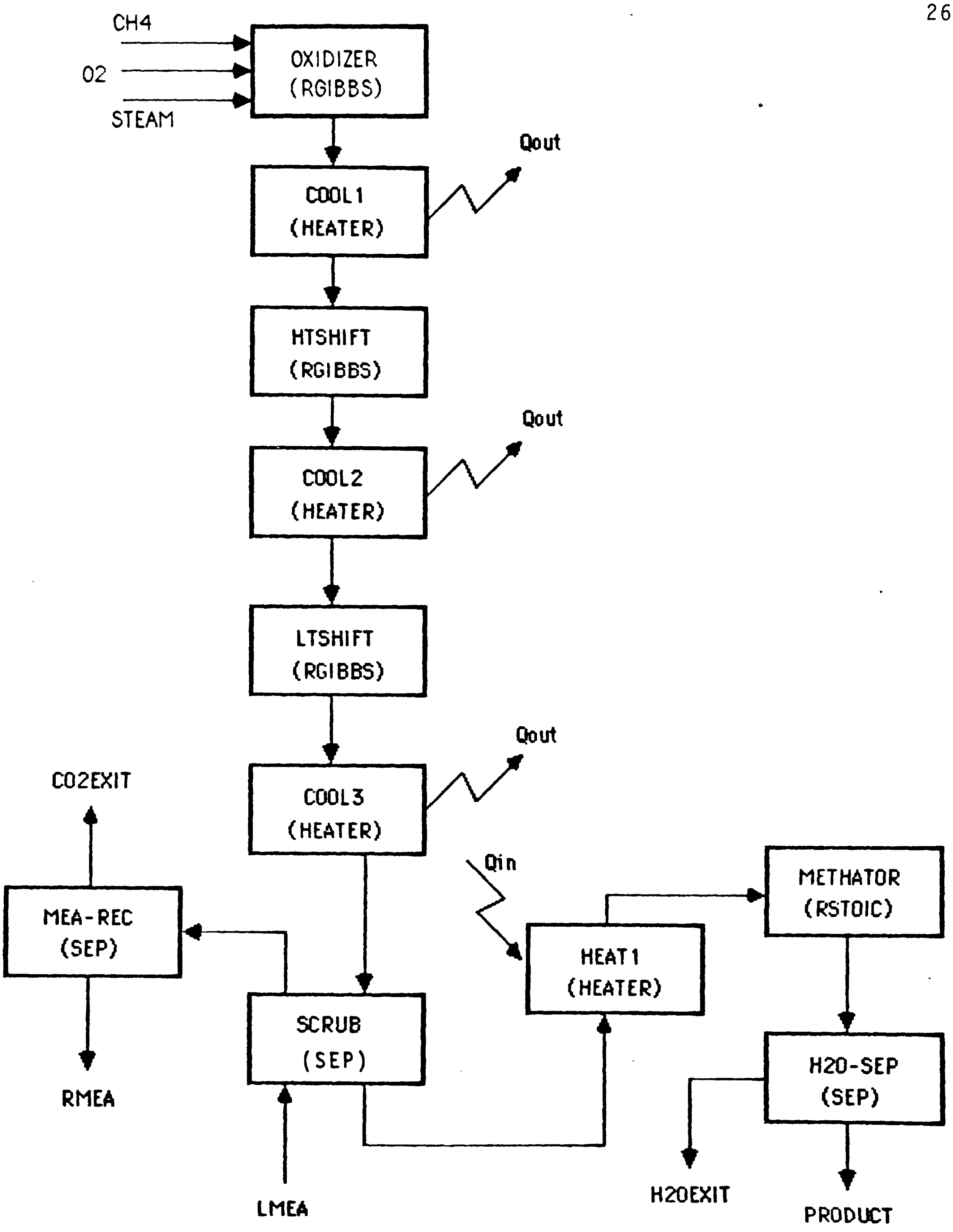


FIGURE 8: ASPEN block diagram for the Partial Oxidation Process

for steam reforming.

ELECTROLYSIS OF WATER

Electrolysis, being a fairly simple process, yields a simple ASPEN block diagram, as seen in Figure 9. Listing 3 in the Appendix shows the ASPEN input language for this simulation. The feed, water, enters the electrolysis cell which is modeled with an "RSTOIC" reactor. Here the stoichiometry of water going to hydrogen and oxygen is specified. Since it has been assumed that all of the feed water is separated, the conversion fraction for this reaction is set at 1.0.

Because only one exit stream is allowed for an "RSTOIC" block, the fact that hydrogen and oxygen are easily separated at the opposite electrodes is modeled with the block "CELLSEP." This is a "SEP" block which takes all of the hydrogen and puts it in one exit stream while taking all of the oxygen and putting it in the other exit stream. Because occasionally liquid water can be entrained with the exit gases, knock-out drums are put in the flowsheet so that the product streams will be pure and dry.

The costing section of the simulation consists primarily of the capital expenditure for the electrolysis cell and the cost of the electricity used. Based on some literature data, the installed capital cost was calculated on the basis of $300 per kw hydrogen heating value. (4)

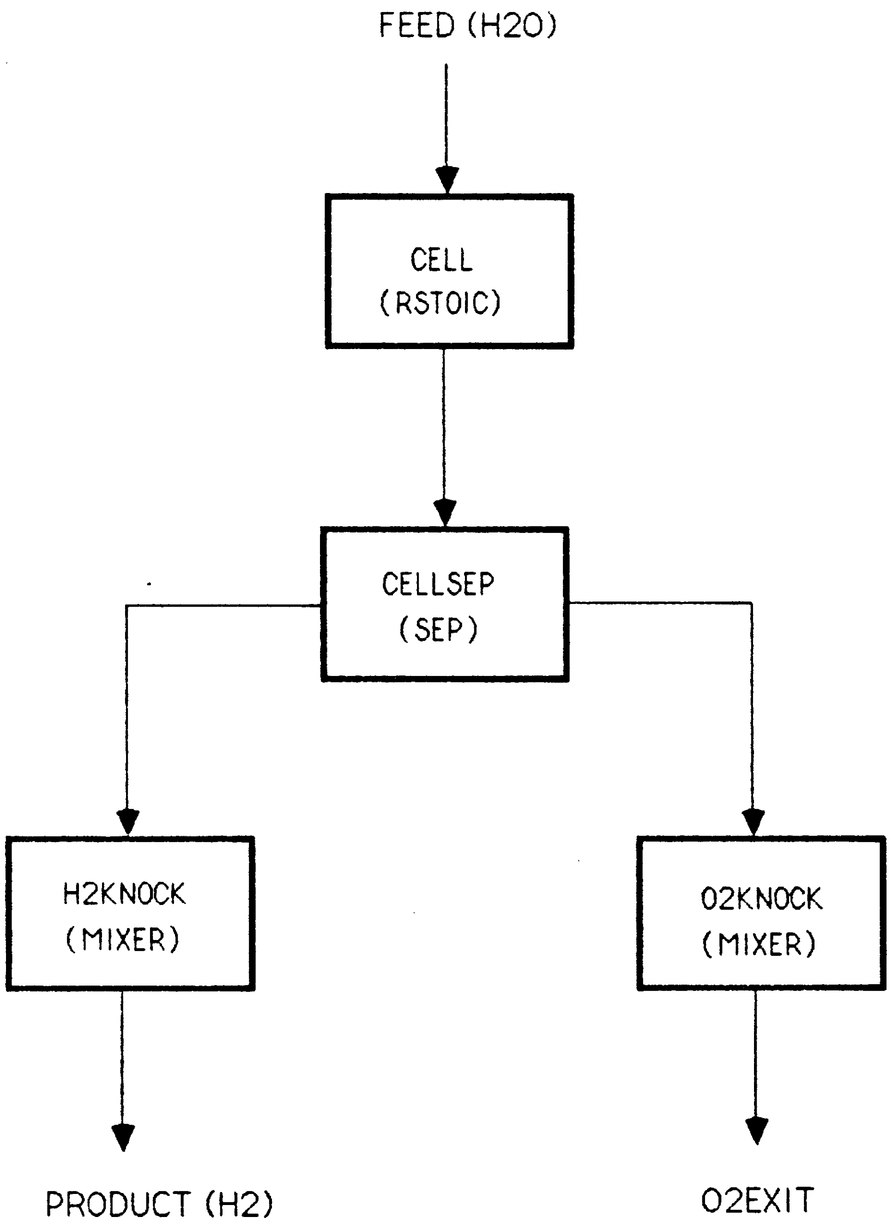


FIGURE 9: ASPEN block diagram for the Electrolysis Process

For the operating cost, no credit was given for the oxygen produced due to the fact that additional investment would be necessary to liquify the oxygen for shipping and it was assumed that there would be no use for oxygen on site.

III. SIMULATION RESULTS

STEAM REFORMING OF METHANE

The simulations developed for these hydrogen production processes have been executed to show some representative results and to demonstrate the potential of flowsheet simulation. There are several ways to measure the performance of a system. First, there is the purity of the product stream. Generally, this stream will consist of hydrogen and methane, and the closer it is to 100% hydrogen the better. Second, there is the hydrogen production rate. If the feed is held constant and the operating conditions varied, not only will the purity change, but the production rate of hydrogen will also change. It might be possible, for example, to run the process in such a way as to get 95% pure hydrogen product while producing at a much lower rate than the potential. This would occur if a great deal of carbon dioxide is produced, which is subsequently removed. So both the purity and production rate are measures of how efficiently the feed is being converted into hydrogen. Also of great importance in measuring the performance of the system is the operating cost per unit of hydrogen produced. This will tell if the plant is cost effective. All of these results will be looked at for the simulations developed.

There are many parameters in the steam reforming process which can be varied to change the performance of the system. Because the reformer reactor is the heart of the system, however, only the operating conditions associated with this unit have been studied. These include the reformer temperature, reformer pressure, and feed steam to methane ratio.

Figure 10 shows the fraction of hydrogen in the process product stream (i.e. the purity - the remaining fraction is all methane) as a function of the reformer temperature. Three curves are shown, each representing a different steam to methane feed ratio. It is clear that as the temperature increases the reformer reactions are driven toward the right, and the purity of the product stream increases. It is interesting to note that the purity approaches 100% under all conditions at temperatures above 1200K. This suggests that operation above 1200K does not gain much and research into higher temperature catalysts and materials is not of great importance.

Figure 10 also shows that the higher the steam to methane ratio, the greater the final purity. Again this is because the excess steam tends to push the methane reaction toward completion.

Figure 11 shows the product stream hydrogen purity versus the reformer pressure. Here the purity drops as the pressure increases, suggesting that higher pressure inhibits the reformer reactions. This is in agreement with

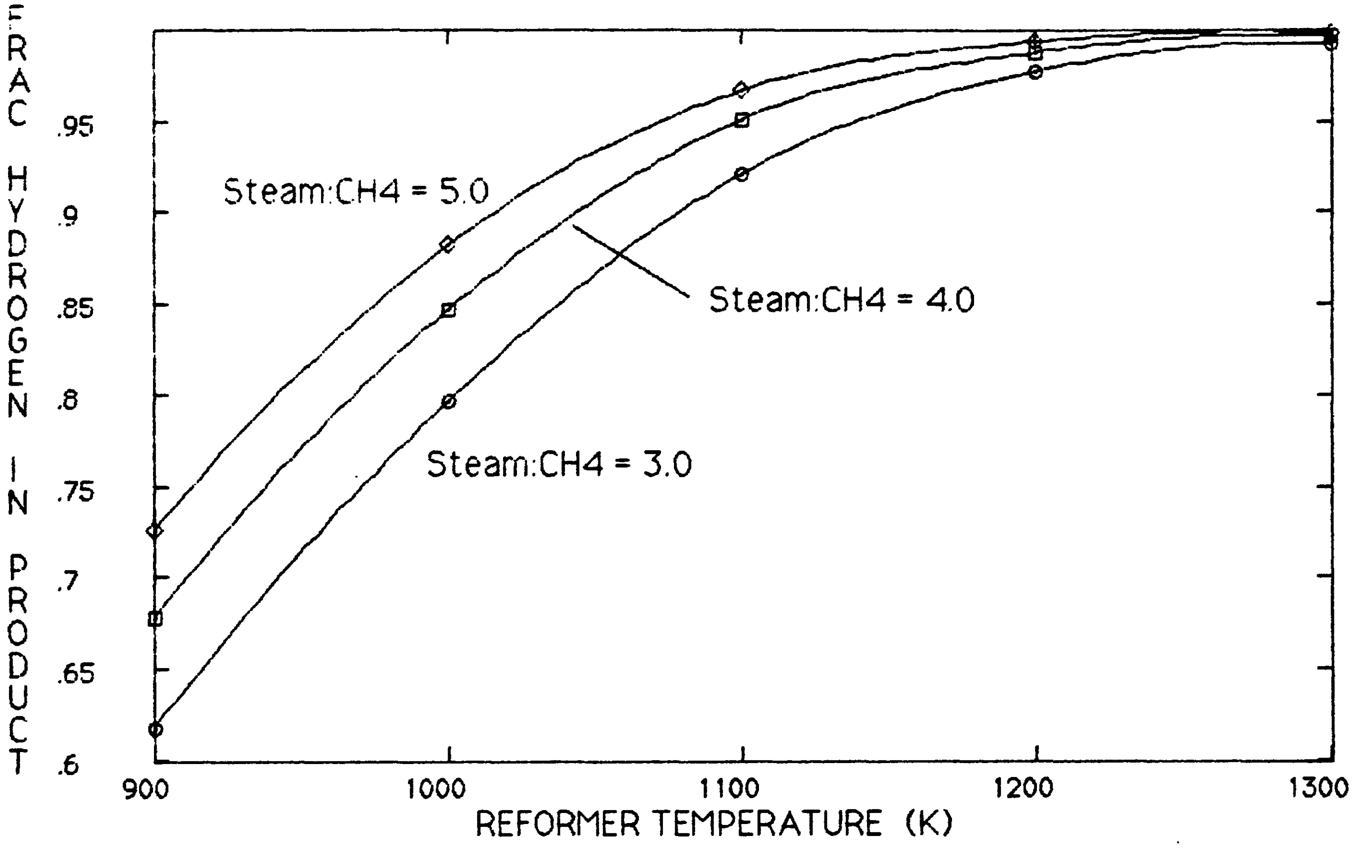


FIGURE 10: Fraction of hydrogen in the steam reforming product stream versus reformer temperature for several steam to methane mole ratios with pressure = 20 ATM

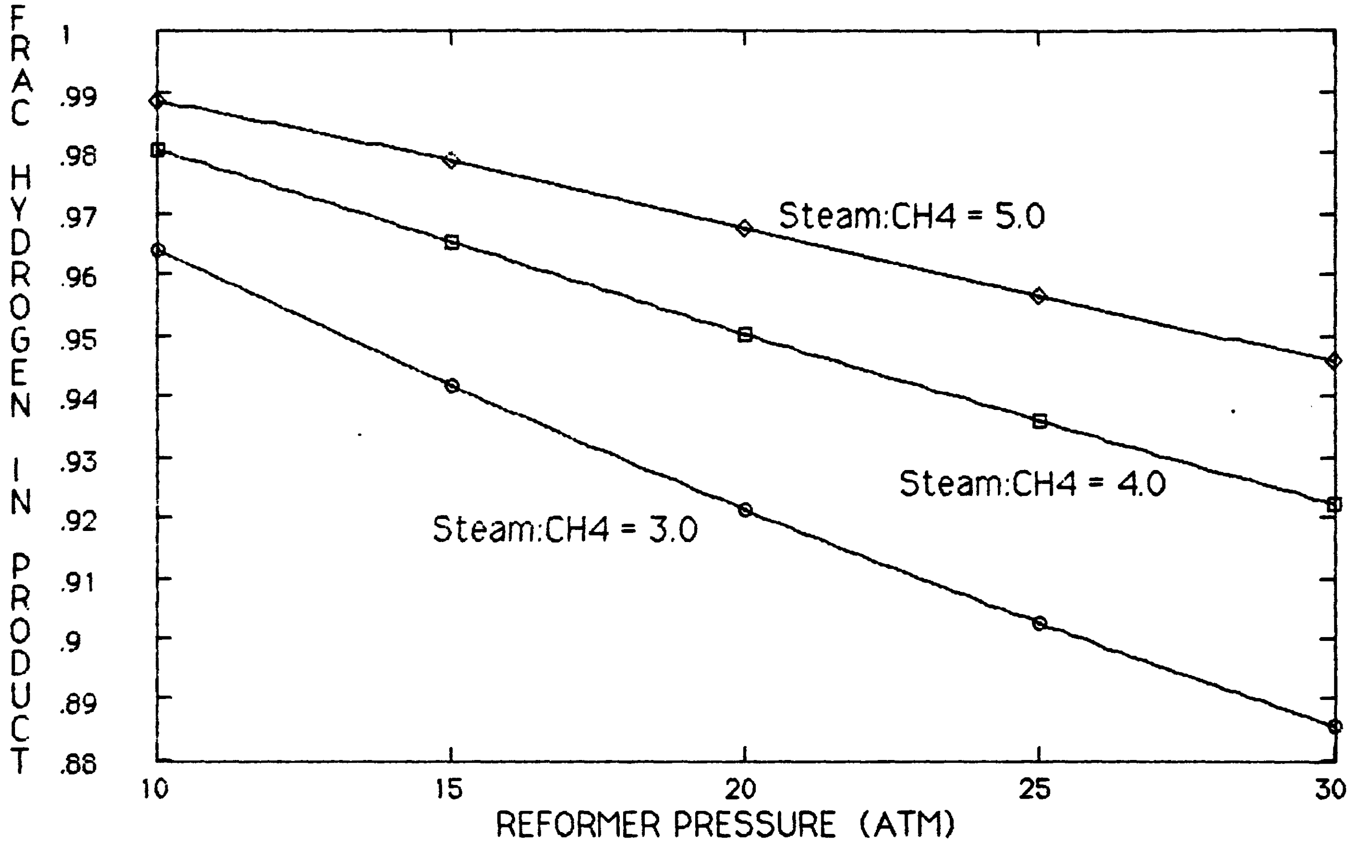


FIGURE 11: Fraction of hydrogen in the steam reforming product stream versus reformer pressure for several steam to methane mole ratios with temperature = 1100K

published literature data. (1) Again the different lines representing different steam to methane feed ratios show that excess steam helps to make the product stream more highly concentrated in hydrogen.

Figure 12 shows the hydrogen production rate from a fixed methane feed versus the reformer temperature. The same trend as observed in Figure 10 is seen here. Higher temperatures favor hydrogen production as do higher steam flow rates.

Figure 13 shows a similar plot for hydrogen production as a function of reformer pressure. It is clear that high pressure comes into direct conflict with high production rates from a given feed. This suggests that the process should be run at low pressure. Indeed, this is often done, however the desirability of high pressure hydrogen at the end of the process becomes a problem. Rather than investing in the compressor necessary to produce this high pressure product, usually the pressure throughout the process is kept high at the sacrifice of production rate. The suitability of one method or the other depends on the required condition of the product stream. For these simulations it has been assumed that pressurized hydrogen is desired (15 ATM or so) and that this pressure is achieved in the process and not with an additional compressor.

Of primary concern in a process such as this is determining the operating conditions which will produce hydrogen in the most cost effective manner. To do this,

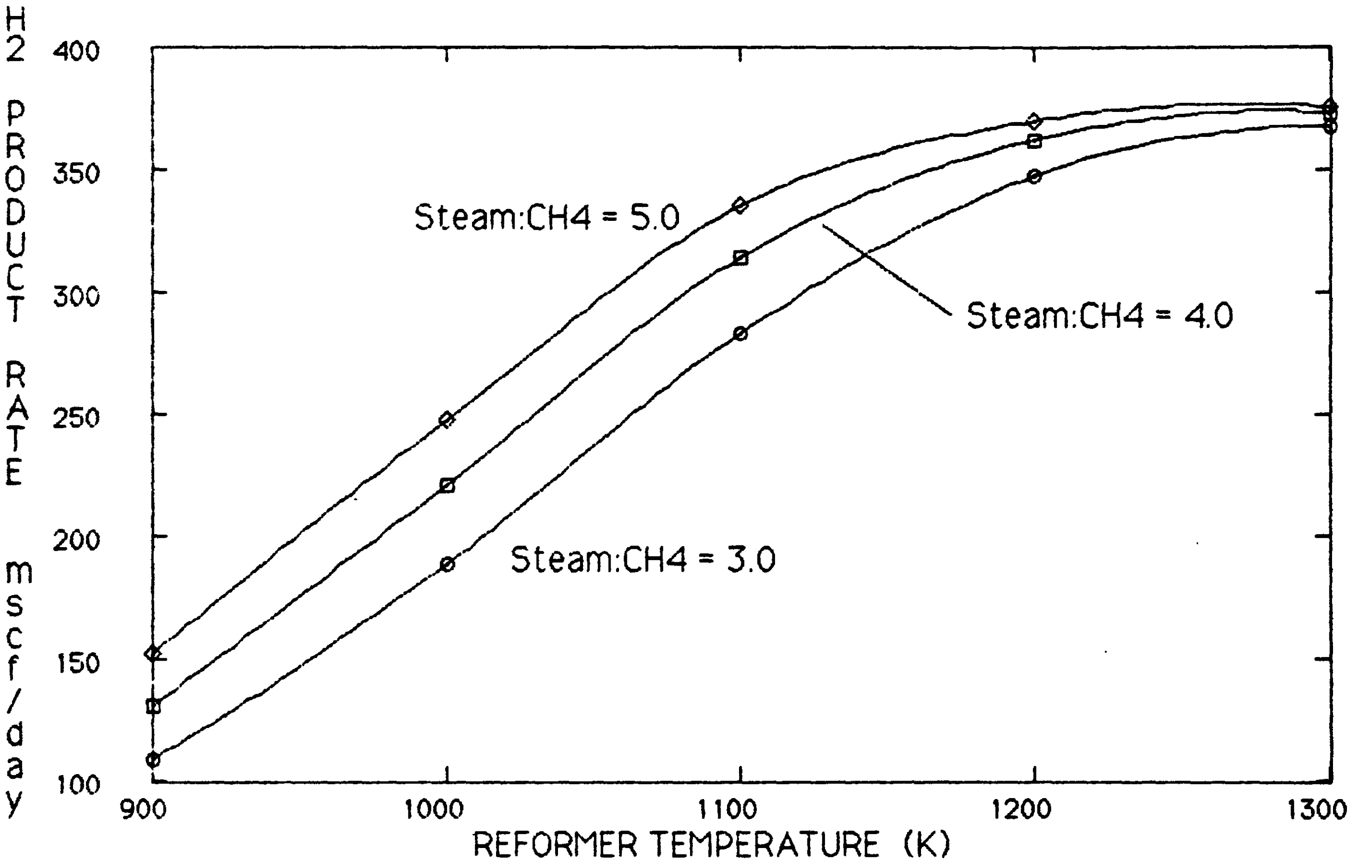


FIGURE 12: Daily hydrogen production rate from the steam reforming process versus the reformer temperature for several steam to methane mole ratios with pressure = 20 ATM

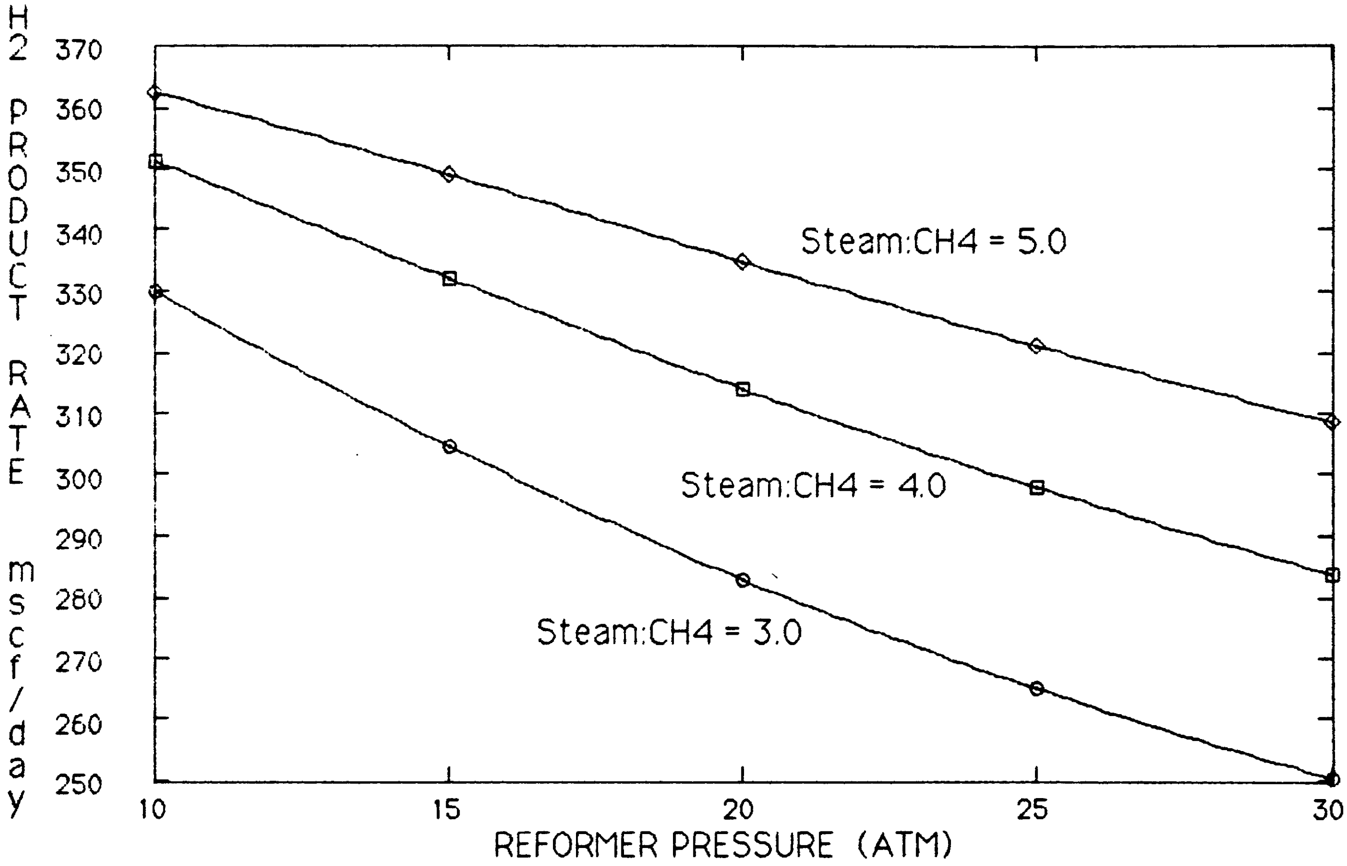


FIGURE 13: Daily hydrogen production rate from the steam reforming process versus the reformer pressure for several steam to methane mole ratios with temperature = 1100K

the cost of hydrogen production is plotted versus each of the operating variables. Figure 14 shows the steam reforming operating cost per million BTU versus the reformer temperature with the pressure set at 20 ATM and the steam to methane ratio at 4.0. The cost drops as temperature increases but reaches an asymptotic limit at about 1100K. With the pressure and steam rate set accordingly, then, the optimum reformer temperature would be about 1100K. In this way the temperature would be the lowest possible while still producing the least expensive hydrogen possible.

Figure 15 shows the hydrogen production cost as a function of the pressure with the temperature set at 1100K and the steam to methane ratio set at 4.0. Because of the decrease in production associated with high pressures, the operating cost rises with pressure. There is no way to look at this curve and select an optimum pressure. As discussed above, the pressure must be selected from a trade-off between cost and necessary exit pressure. For the purposes of this simulation, a value of 20 ATM in the reformer has been assumed to be best - with pressure drops in the process this yields about 14-15 ATM product.

Figure 16 shows the hydrogen cost as a function of the steam to methane ratio with the temperature set at 1100K and pressure set at 20 ATM. At first, as the steam ratio increases, the cost drops. This is because, as observed before, excess steam helps push the methane reaction toward completion. However, above a ratio of

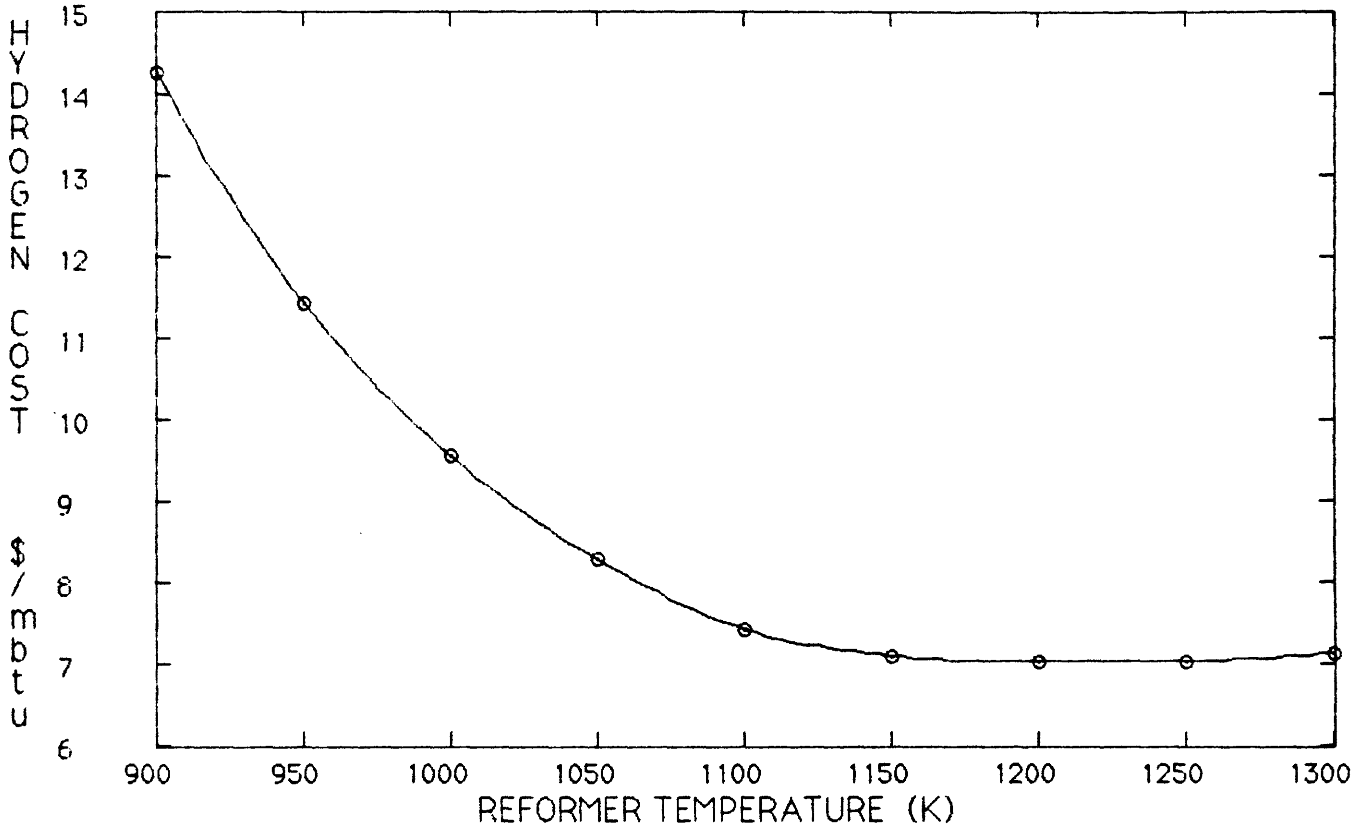


FIGURE 14: Cost of hydrogen produced by the steam reforming process versus the reformer temperature with the reformer pressure = 20 ATM, Steam:CH4 = 4.0

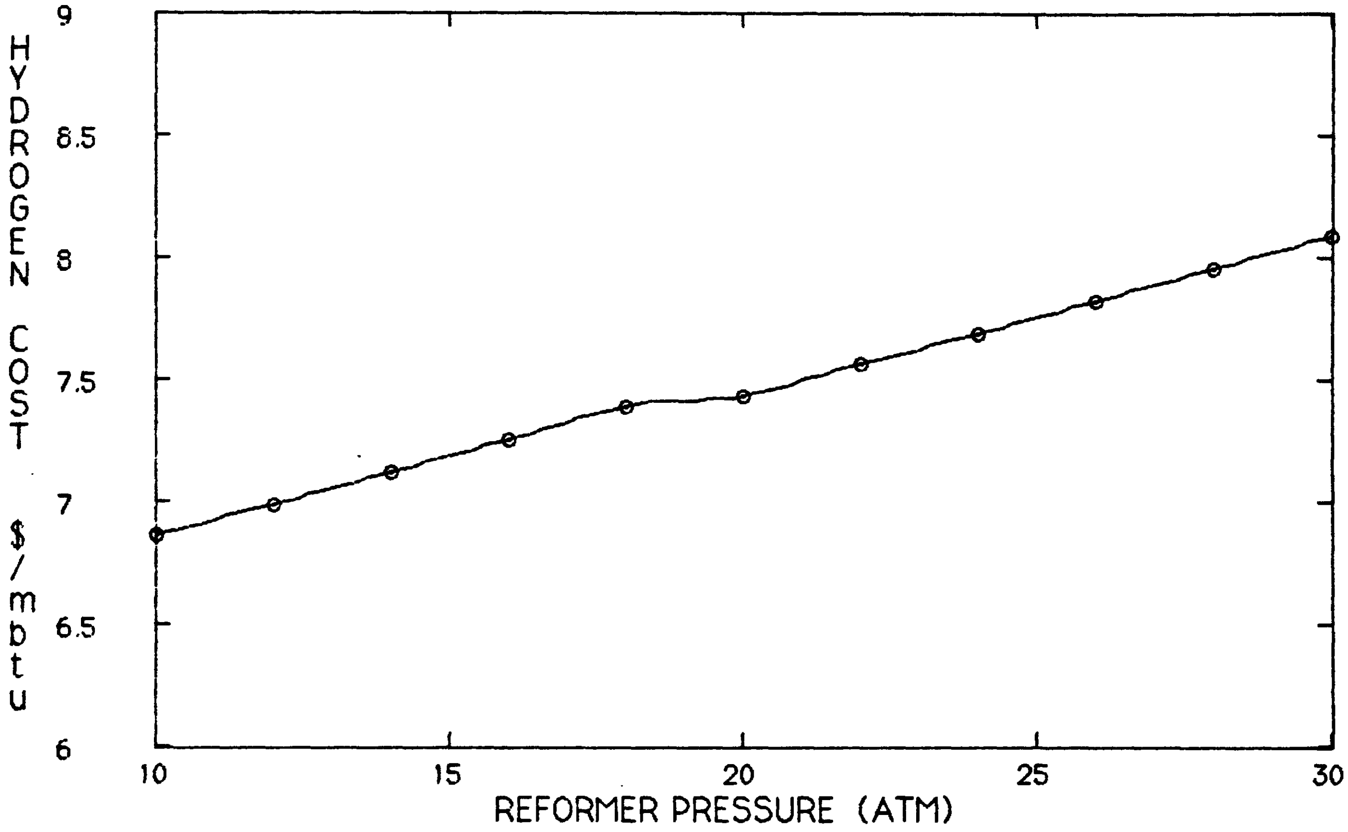


FIGURE 15: Cost of hydrogen produced by the steam reforming process versus the reformer pressure with the reformer temperature = 1100K, Steam:CH4 = 4.0

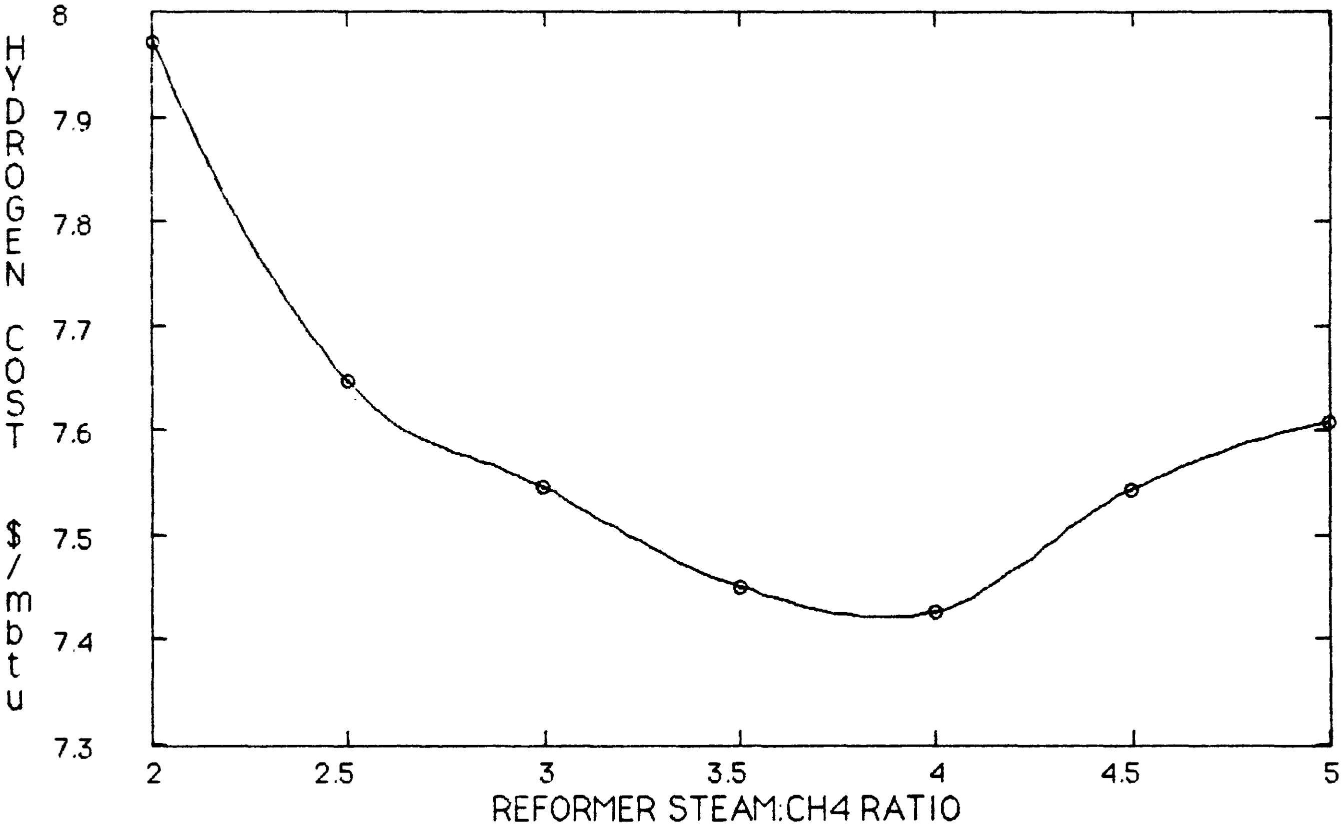


FIGURE 16: Cost of hydrogen produced by the steam reforming process versus the reformer steam:CH4 feed ratio with reformer temp = 1100K, pressure = 20 ATM

about 4.0 the cost begins to rise. This is probably due to the increased purchase cost of the steam and the heating requirements for bringing the incoming steam up to reaction temperatures. The gain associated with excess steam above a ratio of 4.0 is outweighed by the direct operating costs. With the temperature and pressure set as indicated, then, the optimum steam to methane ratio for the reformer feed is 4.0.

It should be emphasized that the optimizations discussed above are reasonably simplified. Each variable was optimized individually with the other two fixed at some value. In a real process, all three would have to be varied simultaneously in order to obtain the overall process optimum.

With the reformer operating conditions set, it is informative to look at a "cross-section" of the process to see what is happening. Figure 17 - obtained with data from a run with the temperature at 1100K, the pressure at 20 ATM, and the steam to methane ratio at 4.0 - shows such a cross-section. The dry mole percent of each species is plotted versus the position in the process.

As indicated, the feed is pure methane. After the reformer, the methane percent has dropped to about 5% and hydrogen is the dominant species at 75%. Carbon monoxide and carbon dioxide are present in about equal concentrations at 10%. In the shift reactors the carbon monoxide is converted to hydrogen and carbon dioxide. Figure 17 shows this, for the carbon monoxide curve drops

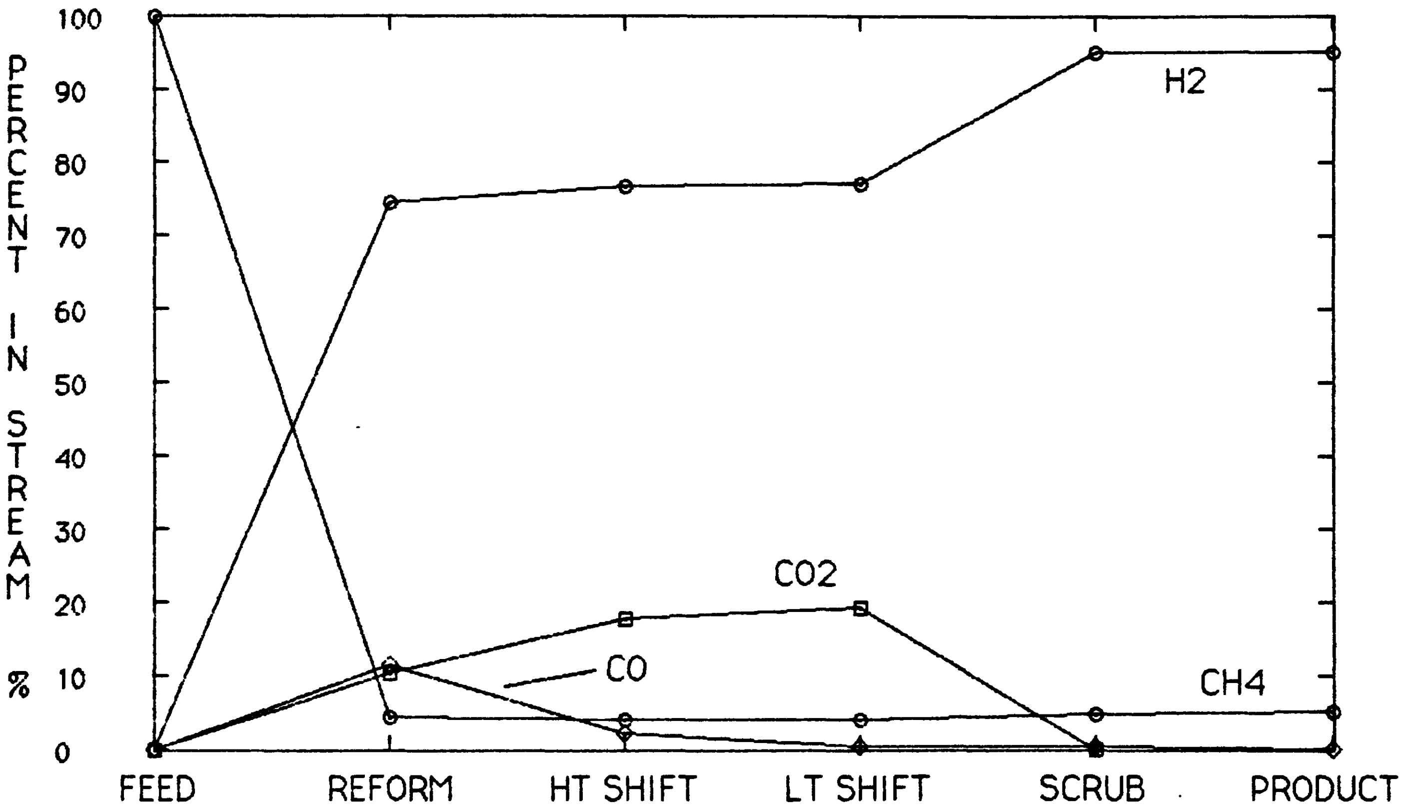


FIGURE 17: Species profile of steam reforming process. The lines show the mole percent of each species in the streams exiting the indicated unit operations

while the carbon dioxide and hydrogen curves rise. Methane stays the same, for it is considered an inert in these reactors.

After the scrubber, the carbon dioxide percent drops to zero, for it has been removed. Because carbon dioxide was acting as a diluent, its removal causes the percentages of all of the other species to rise. The product stream shows the removal of all remaining carbon monoxide by the methanator. The resulting product consists of 95% hydrogen and 5% methane.

It is well known that different size plants will perform economically differently. As a final look at the steam reforming process, it is informative to look at the hydrogen cost as a function of the plant capacity. Figure 18 show such a plot. Because of the wide range of plant sizes covered (10 mscf/day to 300 mscf/day) three distinct areas emerge on this plot. At low capacity, a sharp economy of scale is observed. There are minimum sizes for units such as reformer furnaces, and if the process is run below the limits of these units, it will be very expensive (high capital and operating cost spread over low production rates). Thus the cost drops as the size increases for low production rates.

In the center of the figure, a relatively flat region is observed. Here the process is being run at rates easily handled by the equipment available. Increasing production simple increases the capital and operating costs proportionately, and the resultant hydrogen cost stays

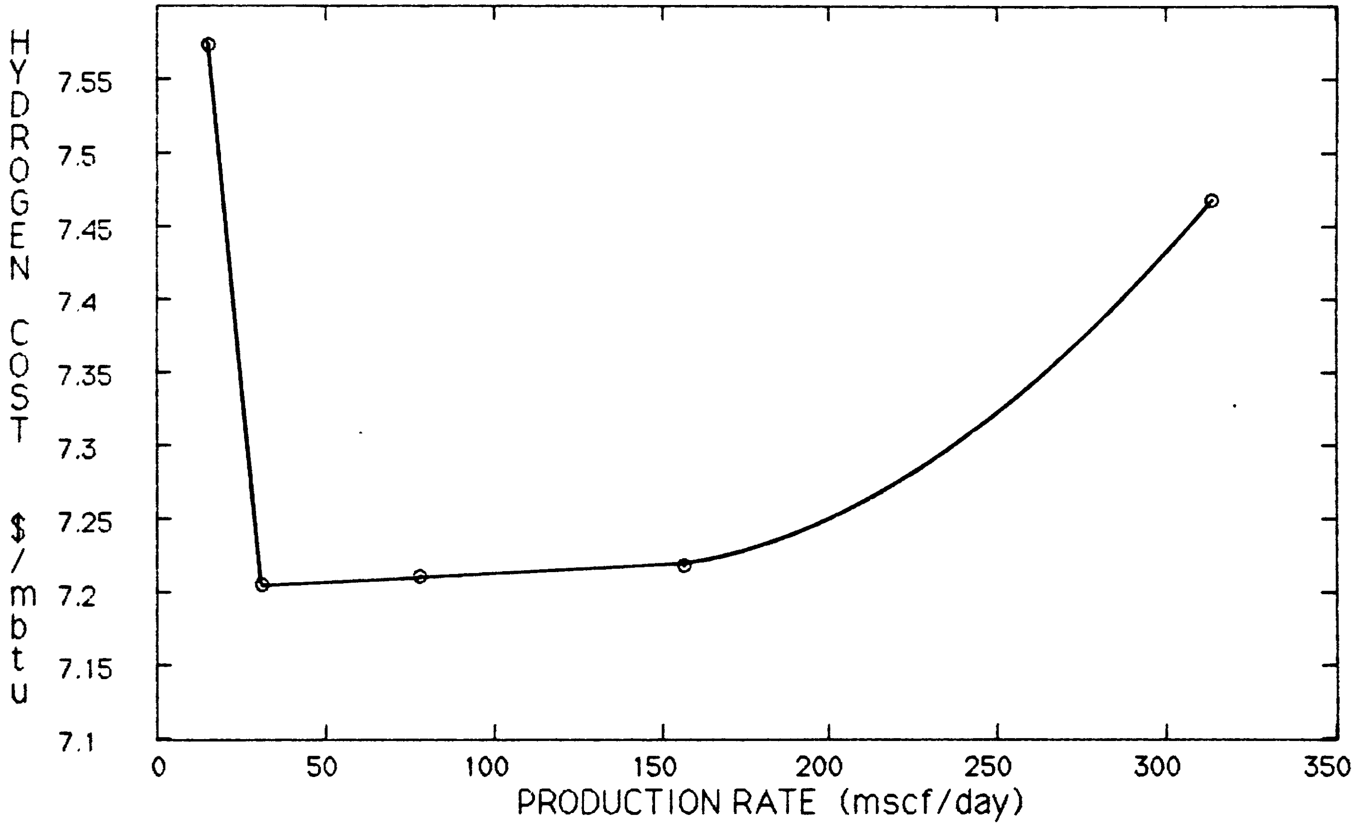


FIGURE 18: Cost of hydrogen produced by the steam reforming process versus the plant capacity with the reformer temp = 1100K, pressure = 20 ATM, steam:CH4 = 4.0

about the same.

At high production rates, however, larger and larger pieces of equipment are necessary. As equipment size increases, the costs tend to rise more quickly. Thus at high production rates the costs are increasing faster than the hydrogen produced, and the unit cost begins to rise.

As a basis of comparison with the other processes, the actual cost figures for a selected plant size have been summarized. Figure 19 shows this summary. As indicated, a medium size facility of 300 mscf/day was used. The reformer operating conditions are indicated. The total operating cost was found to be $7.43 per million BTU of hydrogen which is in agreement with some representative literature data. (9) As the pie chart indicates, the major pieces of the operating cost are raw materials (e.g. methane and feed steam costs) and utilities (e.g. fuel oil and cooling water). The remainder of the cost is split fairly evenly between labor, overhead, and capital depreciation.

Also shown in Figure 19 is the capital investment required for a steam reforming plant this size. The total bill would be about $300 million, split between process unit purchase costs, setting labor, other directs such as land, contingency, working capital, and start-up costs.

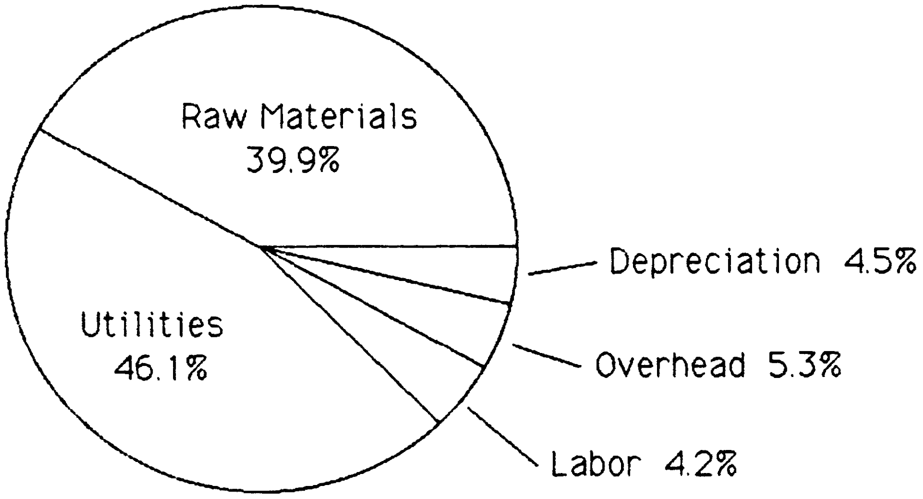
PLANT CAPACITY: 300 million scf per day

OPERATING PARAMETERS:

Reformer Temperature = 1100K
Reformer Pressure = 20 ATM
Steam:CH4 = 4.0

OPERATING COST = $ 7.43 per million btu hydrogen

OPERATING COST BREAKDOWN:



CAPITAL COST SUMMARY:

Process Units	$ 69,901,000
Other Directs	34,885,000
Setting Labor	50,953,000
Contingency	45,538,000
Working Capital	75,223,000
Start up Cost	55,816,000
TOTAL:	$ 332,316,000

FIGURE 19: Operating and capital cost breakdowns for a 300 mscf per day hydrogen plant using steam reforming

PARTIAL OXIDATION OF METHANE

A similar analysis of the partial oxidation process has been made. In this way, it is possible to compare steam reforming with partial oxidation. Again many operating parameters in this process can be changed to affect the system performance. As with the reformer, this study concentrates only on those operating conditions associated with the primary reactor: the oxidizer. These operating parameters include the oxidizer temperature, pressure, oxygen to methane feed ratio, and steam to methane feed ratio. To limit the scope slightly, the steam to methane ratio was set at 1.0 throughout to eliminate this variable. The performance of the system was studied as a function of the remaining three operating conditions.

Figure 20 shows the hydrogen product purity as a function of the oxidizer temperature. The three curves represent different oxygen to methane feed ratios. As with the reformer, as the temperature increases the purity rises. They all begin to reach an asymptotic limit at a temperature slightly over 1100K. This graph also indicates that the higher the oxygen to methane ratio, the higher the purity of the product stream. This is because excess oxygen drives the methane reaction to the right, eliminating the methane from subsequent process streams.

Figure 21 shows the hydrogen product purity as function of the oxidizer pressure. As with the reformer, higher pressure tends to inhibit the reactions, decreasing

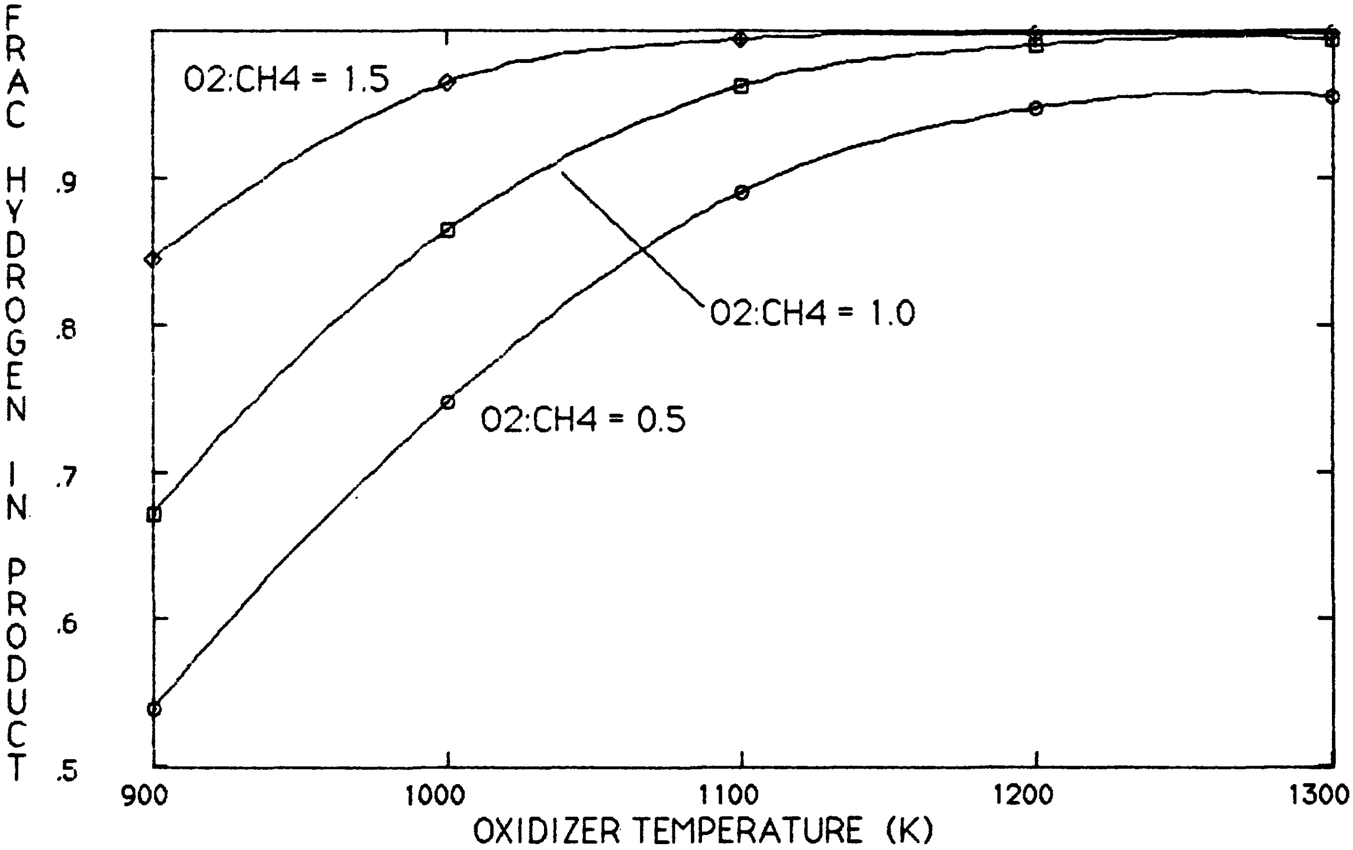


FIGURE 20: Fraction of hydrogen in the partial oxidation product stream versus the oxidizer temperature for several oxygen to methane mole ratios with pressure = 20 ATM

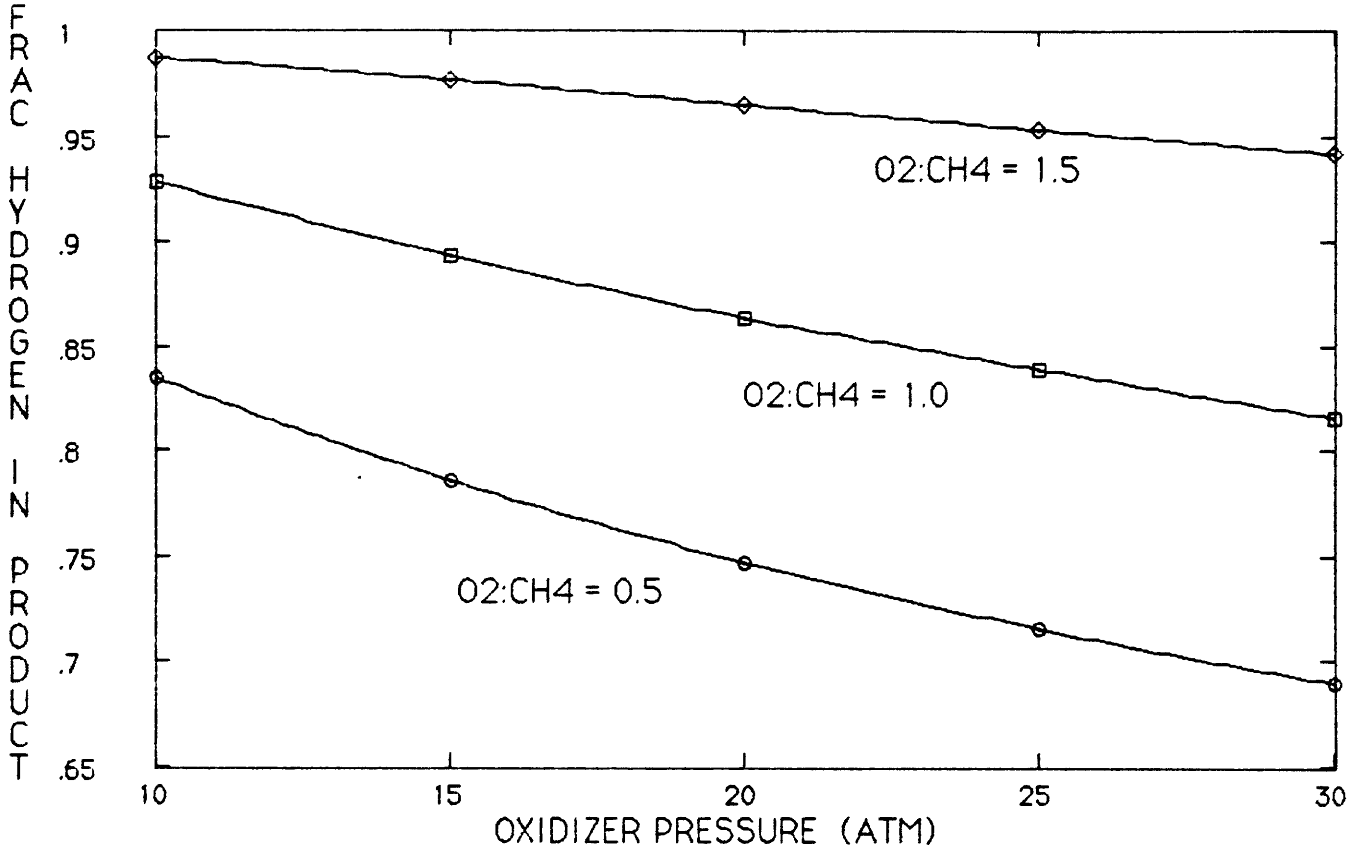


FIGURE 21: Fraction of hydrogen in the partal oxidation product stream versus the oxidizer pressure for several oxygen to methane mole ratios with temperature = 1100K

the concentration of hydrogen in the product. This graph suggests that higher oxygen to methane ratios not only produce more pure product, but also tend to limit the adverse effects of the higher pressures (compare the slope of the $O2:CH4=1.5$ line with the $O2:CH4=0.5$ line).

Figure 22 shows the total hydrogen production rate versus the oxidizer temperature. The production rate increases then begins to level off at some point. This shows that similar to the reformer process there is no great advantage to using temperatures above about 1200K for partial oxidation. It is important to note that this figure shows that low oxygen to methane feed ratios yield a higher production rate from a set methane feed. This is one of those cases in which the product purity conflicts with the production rate (compare Figures 20 and 22). Excess oxygen forces more methane to react, increasing the purity, but this same excess oxygen causes full oxidation to take place, burning up some of the desired hydrogen.

Figure 23 shows a similar plot for hydrogen production rate versus oxidizer pressure. Increasing the pressure drops the production rate. This highlights again the conflict between production rate and desired product pressure. Also shown is a confirmation of the fact that higher oxygen to methane feed ratios give lower production rates.

The effect of the operating conditions on the hydrogen cost will now be examined. Figure 24 shows the hydrogen cost per million BTU versus the oxygen to methane

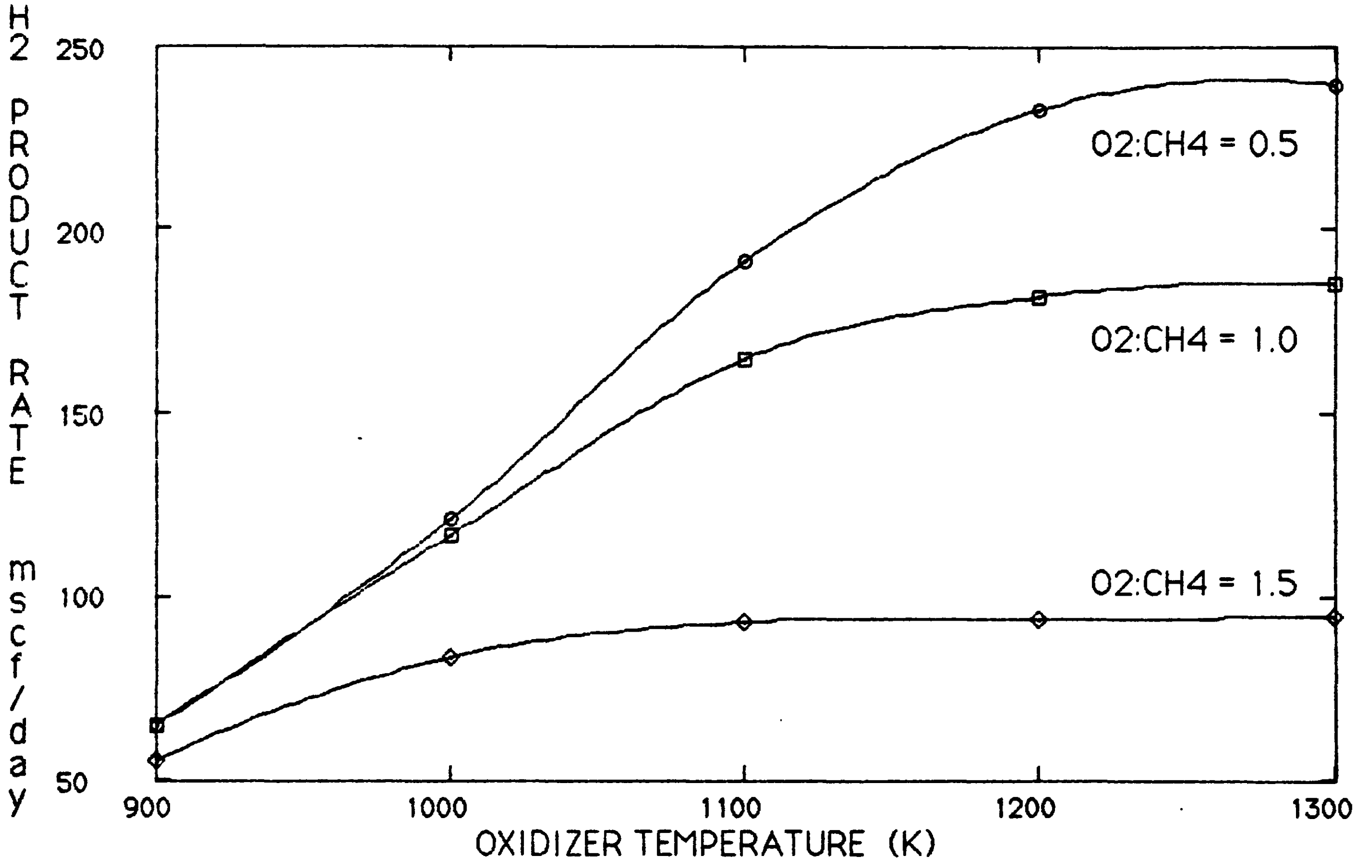


FIGURE 22: Daily hydrogen production rate from the partial oxidation process versus the oxidizer temperature for several oxygen to methane mole ratios with pressure = 20 ATM

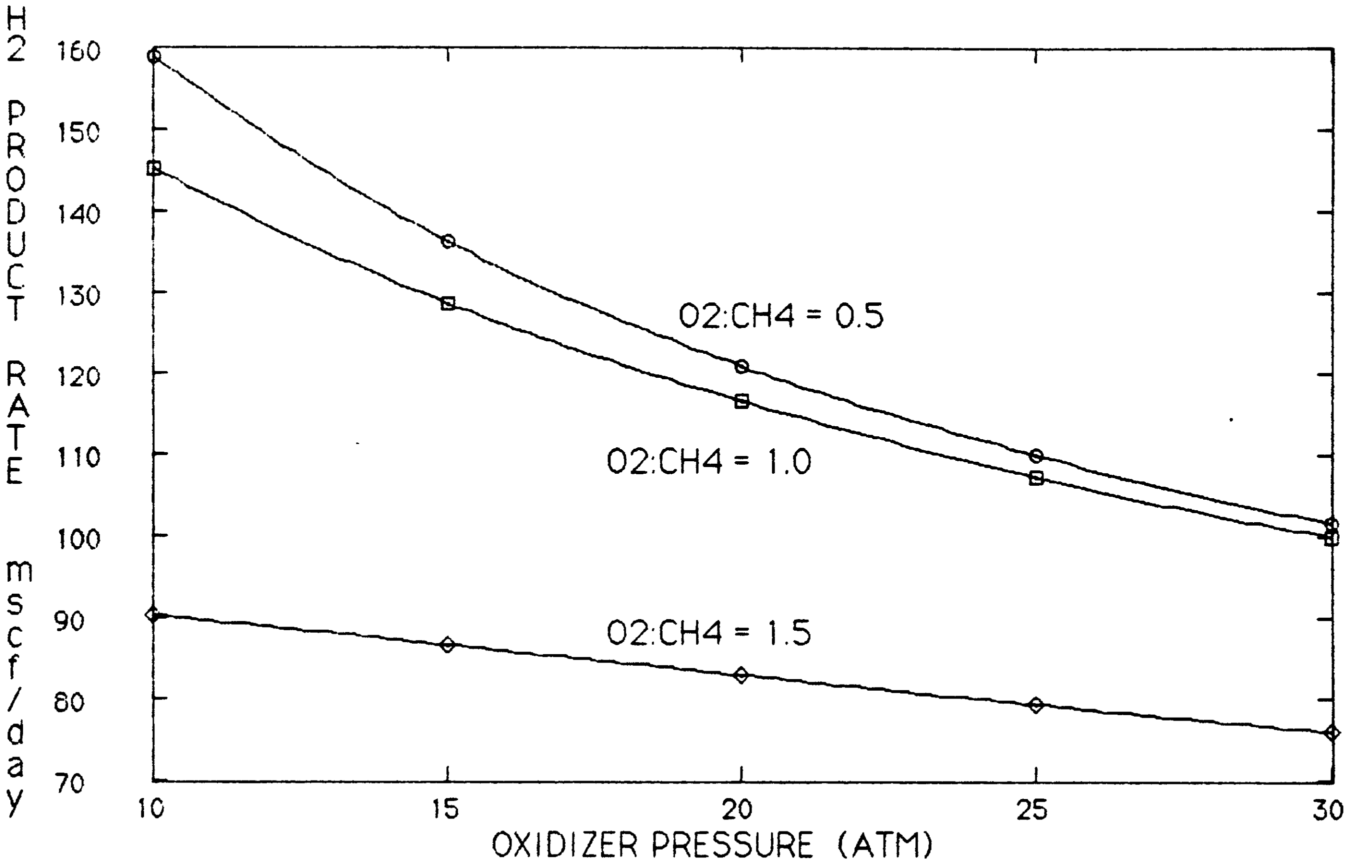


FIGURE 23: Daily hydrogen production rate from the partial oxidation process versus the oxidizer pressure for several oxygen to methane mole ratios with temperature = 1100K

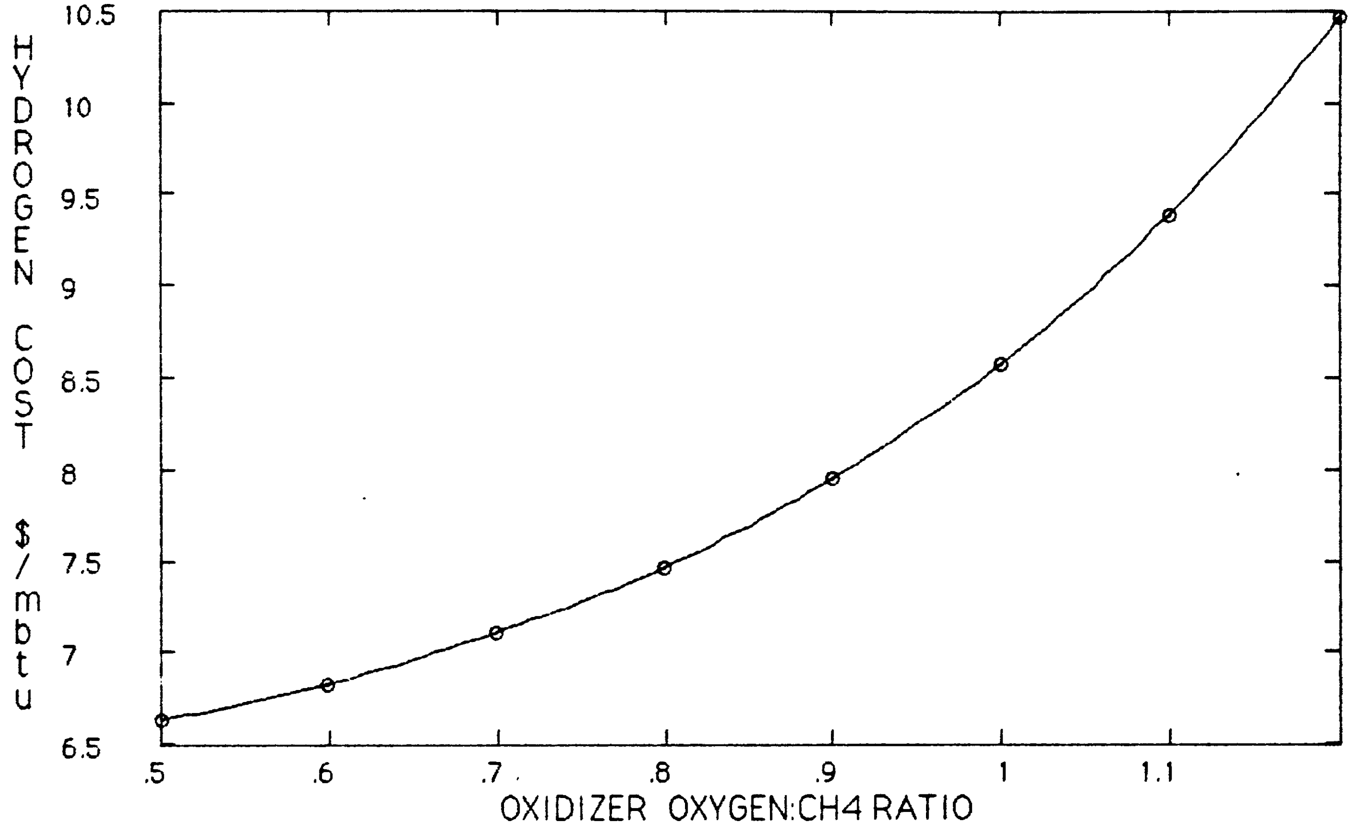


FIGURE 24: Cost of hydrogen produced by the partial oxidation process versus the oxidizer oxygen:CH4 feed ratio with oxidizer temp=1100K, pressure=20 ATM

feed ratio with the temperature set at 1100K and the pressure set at 20 ATM. Because of decreasing production rates, increasing the oxygen to methane ratio increases the hydrogen cost. This is also in part due to the increasing cost of the oxygen which must be supplied to the oxidizer. There is no way to select an optimum ratio from this curve. There is a trade-off between cost and desired product purity which can only be solved when the purity is specified. In order to compare to the results from the steam reforming process, the desired purity was set at about 95%. Based on this, for the given temperature and pressure, the necessary oxygen to methane ratio is 1.0 (see Figure 20).

Figure 25 shows the hydrogen cost as a function of the oxidizer temperature with the oxygen to steam ratio set at 1.0 and the pressure set at 20 ATM. The cost drops as the temperature increases and then levels off. As with the reformer process, the optimum temperature was taken as the lowest at which the cost is a minimum. From Figure 25 this optimum oxidizer temperature is seen to be about 1100K.

Figure 26 shows the hydrogen cost versus the oxidizer pressure. The cost rises steadily as the pressure increases. Again, an optimum cannot be determined without a specification of the desired product pressure. For comparison with the reformer process, an oxidizer pressure of 20 ATM was selected.

Figure 27 shows a cross-section of the partial oxidation process similar to that presented for steam

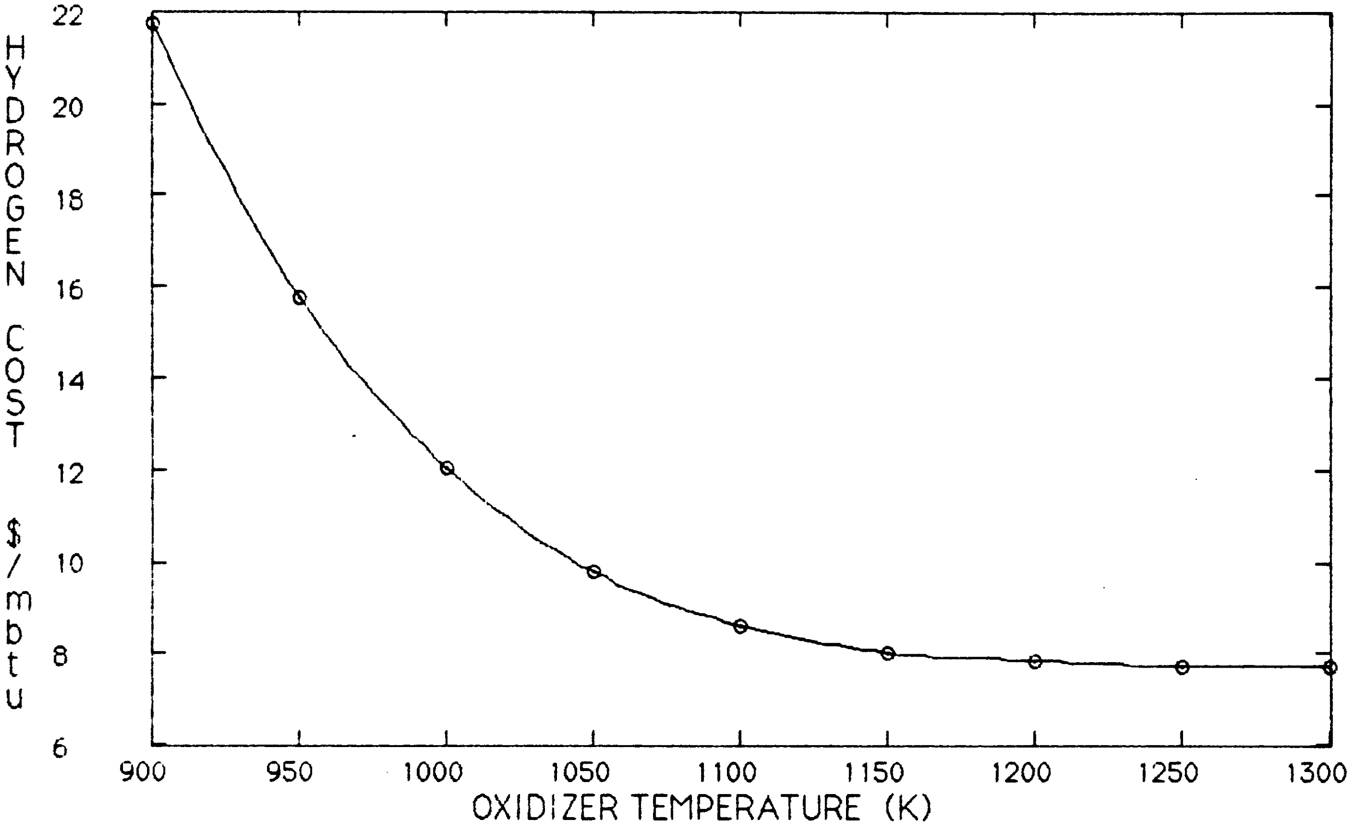


FIGURE 25: Cost of hydrogen produced by the partial oxidation process versus the oxidizer temperature with oxidizer pressure=20 ATM, O2:CH4 = 1.0

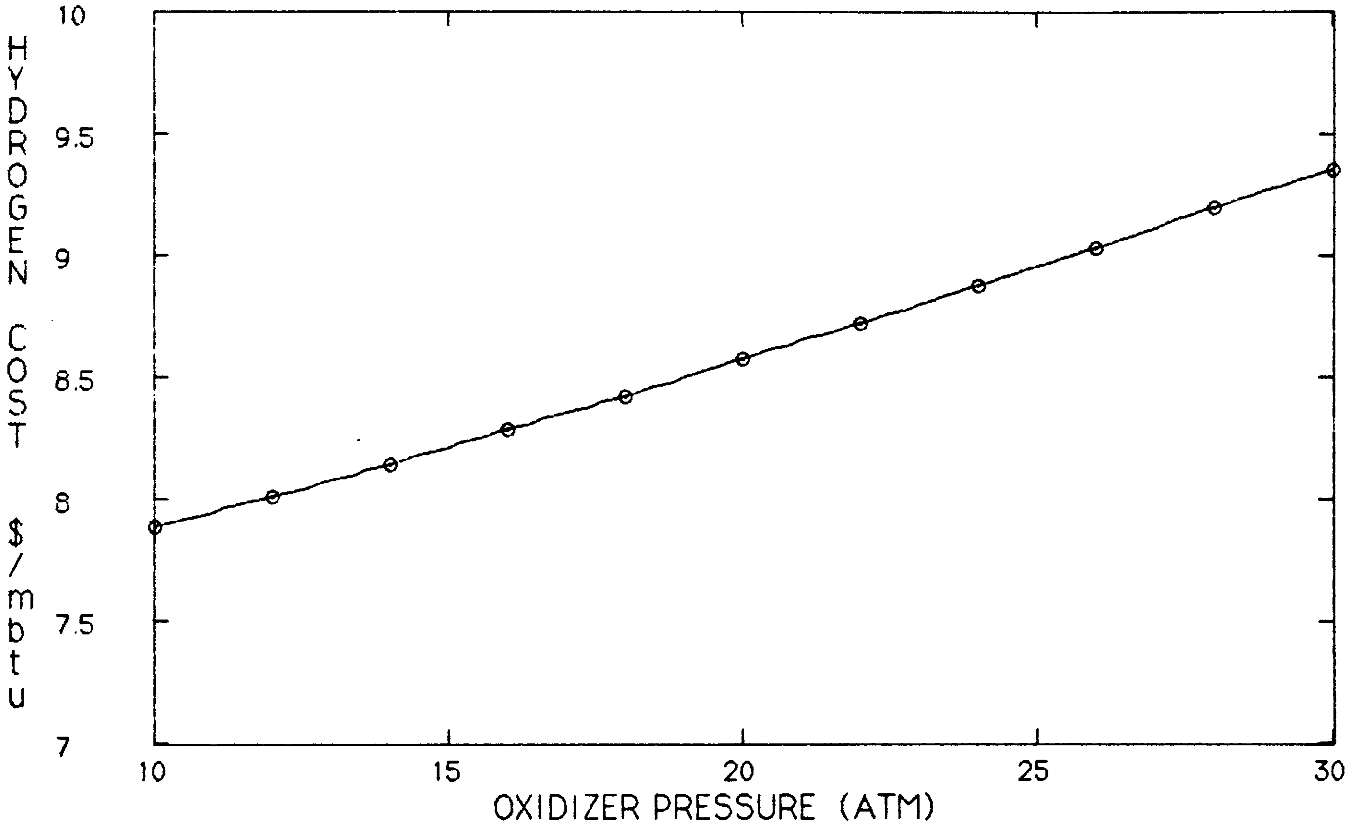


FIGURE 26: Cost of hydrogen produced by the partial oxidation process versus the oxidizer pressure with the oxidizer temp=1100K, O2:CH4 = 1.0

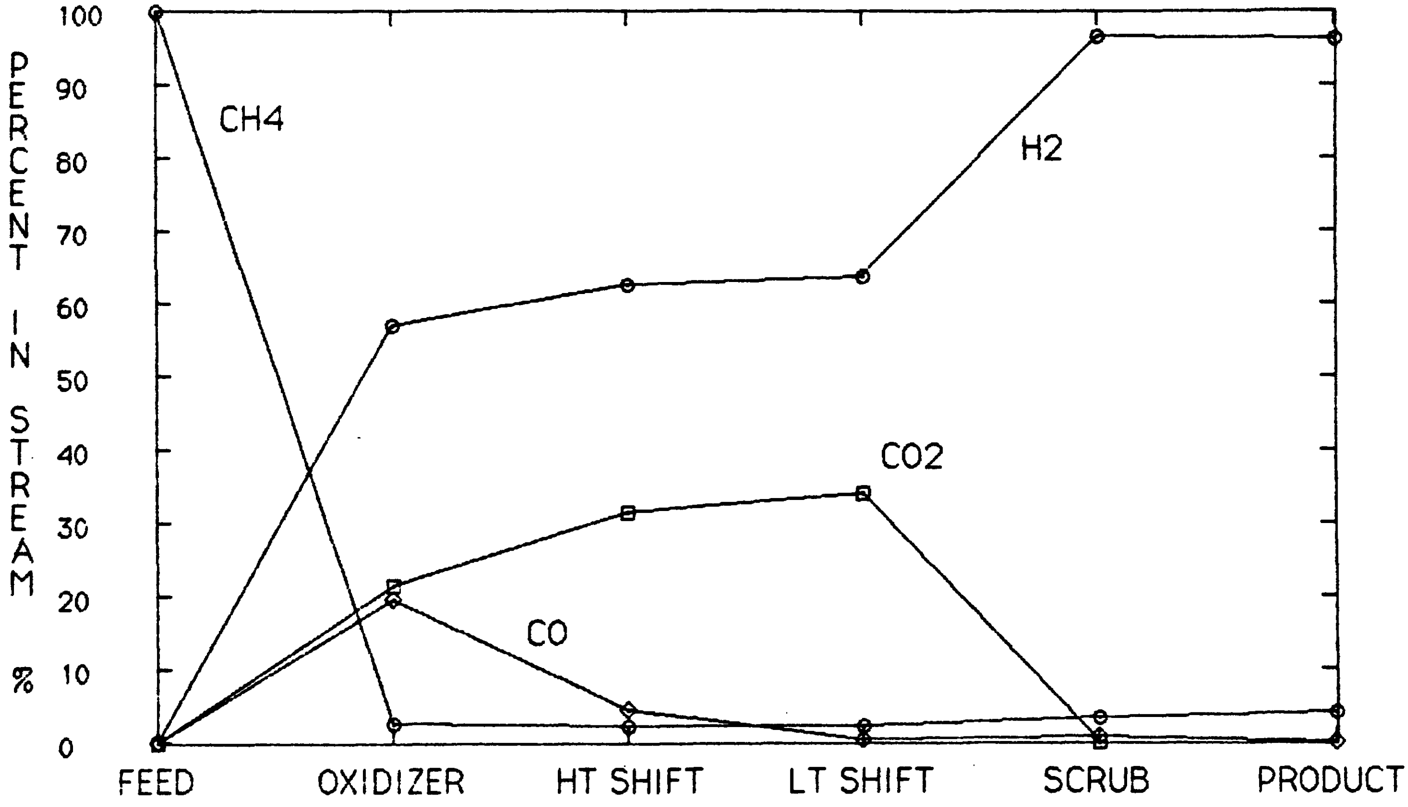


FIGURE 27: Species profile of partial oxidation process. The lines show the mole percent of each species in the streams exiting the indicated unit operations

reforming. The feed is pure methane, and after the oxidizer the methane concentration drops to less than 5% on a dry mole basis. The carbon monoxide and carbon dioxide concentrations are about equal at 20%. Oxygen is not shown, for it was found to completely react in the oxidizer. This leaves hydrogen at about 57%. Comparing this to the steam reforming result shows that more carbon oxides are formed in this process, yielding less hydrogen from the primary reactor.

The two shift reactors show the carbon monoxide being almost completely converted to carbon dioxide and hydrogen. The scrubber removes all of the carbon dioxide, and the methanator reacts the trace amounts of carbon monoxide. The final product stream, as desired, is about 95% hydrogen and 5% methane.

Figure 28 shows the cost of the hydrogen as a function of the plant capacity. Three curves are shown, each representing a different oxygen purchase cost. It has been suggested that the primary reason steam reforming is favored over partial oxidation is because of the investment necessary to produce the oxygen. (11) This investment can be translated into the oxygen purchase cost in order study the effect of this cost on the viability of the process. As would be expected, this graph shows that cheaper oxygen produces a cheaper hydrogen product. These curves will be compared to the one from steam reforming later in this section.

The same general cost trends as those observed in

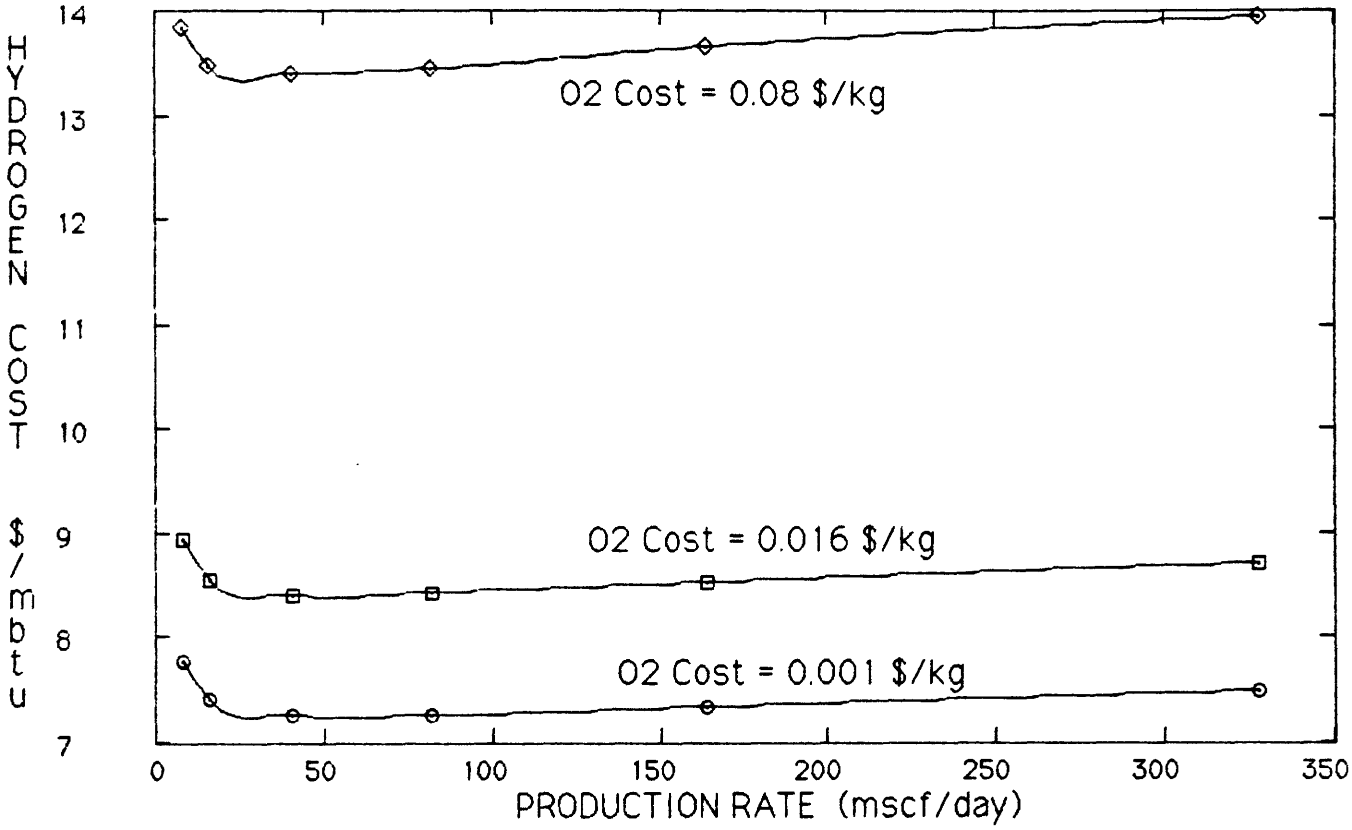


FIGURE 28: Cost of hydrogen produced by the partial oxidation process versus the plant capacity for several oxygen purchase costs with oxidizer temp=1100K, pres=20 ATM, O2:CH4 = 1.0

steam reforming are seen in Figure 28. At low production rate there is a sharp economy of scale. Yet as production increases, the costs rise faster than the capacity and the hydrogen cost slowly rises.

The operating and capital costs for a 300 mscf/day partial oxidation plant have been tabulated in Figure 29. The operating conditions are shown and the operating cost is seen to be \$8.74 per million BTU hydrogen - about \$1.30 more expensive than steam reforming. The operating cost breakdown is quite different for this process than that of steam reforming. The major cost is raw materials and utilities take up less of the cost. This is because in partial oxidation the heat in the primary reactor is supplied by the feed oxygen (a raw material) while in steam reforming the heat is supplied externally by burning fuel oil (a utility).

Figure 29 also shows the capital investment summary for a partial oxidation plant of this size. The total investment would be about \$186 million - \$150 million lower than the steam reforming process. The fact that the capital is lower for partial oxidation is in large part due to the fact that the primary reactor is far less complicated, requiring a lower purchase , setting, and start-up cost.

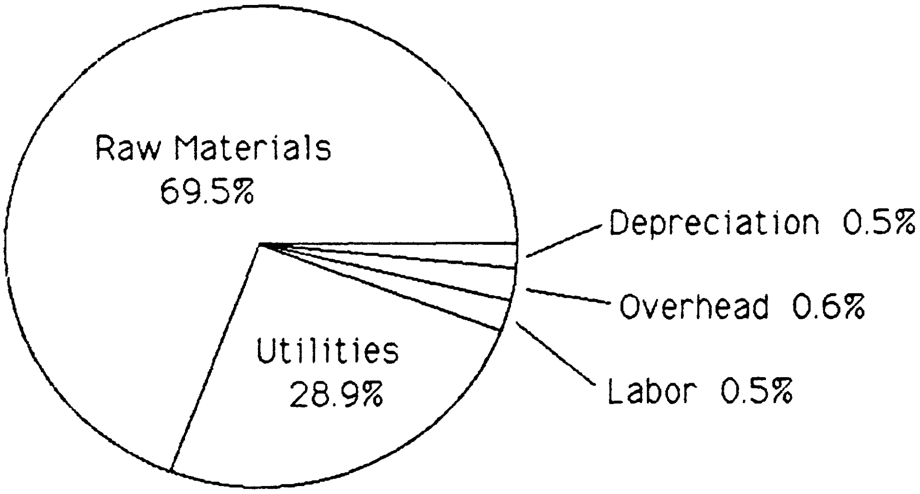
PLANT CAPACITY: 300 million scf per day

OPERATING PARAMETERS:

Oxidizer Temperature = 1100K
Oxidizer Pressure = 20 ATM
Oxygen:CH4 = 1.0
Steam:CH4 = 1.0

OPERATING COST = $ 8.74 per million btu hydrogen

OPERATING COST BREAKDOWN:



CAPITAL COST SUMMARY:

Process Units	$ 10,937,000
Other Directs	4,924,000
Setting Labor	6,120,000
Contingency	6,427,000
Working Capital	96,225,000
Start up Cost	62,005,000
TOTAL:	$ 186,638,000

FIGURE 29: Operating and capital cost breakdowns for a 300 mscf per day hydrogen plant using partial oxidation

ELECTROLYSIS OF WATER

In the electrolysis simulation there are no real operating conditions which can be varied. Although the temperature and pressure can have some effect on the cell efficiency (4), for simplicity the cell efficiency in this simulation was assumed constant at 85%. The only operating parameter of interest, then, is the hydrogen production rate versus the feed flow rate. Figure 30 shows this relationship. As would be expected, the production increases linearly with the water feed rate. This graph can be used to find the necessary water feed rate given a desired production rate.

Figure 31 shows the cost performance of this process. In the oxidation process the price of oxygen was the key cost factor. Here the cost of electricity is critical. The three curves shown in Figure 31 represent different electricity purchase prices. In all cases the cost of hydrogen increases with the plant capacity because of the accelerating cost of high capacity electrolysis cells. It is interesting to note that no economy of scale is observed at low production rate. This is because unlike reformer or oxidizer reactors, electrolysis units do not really have a minimum size. As expected, the lower the cost of electricity, the lower the product hydrogen cost.

Figure 32 shows the operating and capital cost breakdowns for an electrolysis plant producing 300 mscf/day hydrogen. The necessary feed rate is shown and the

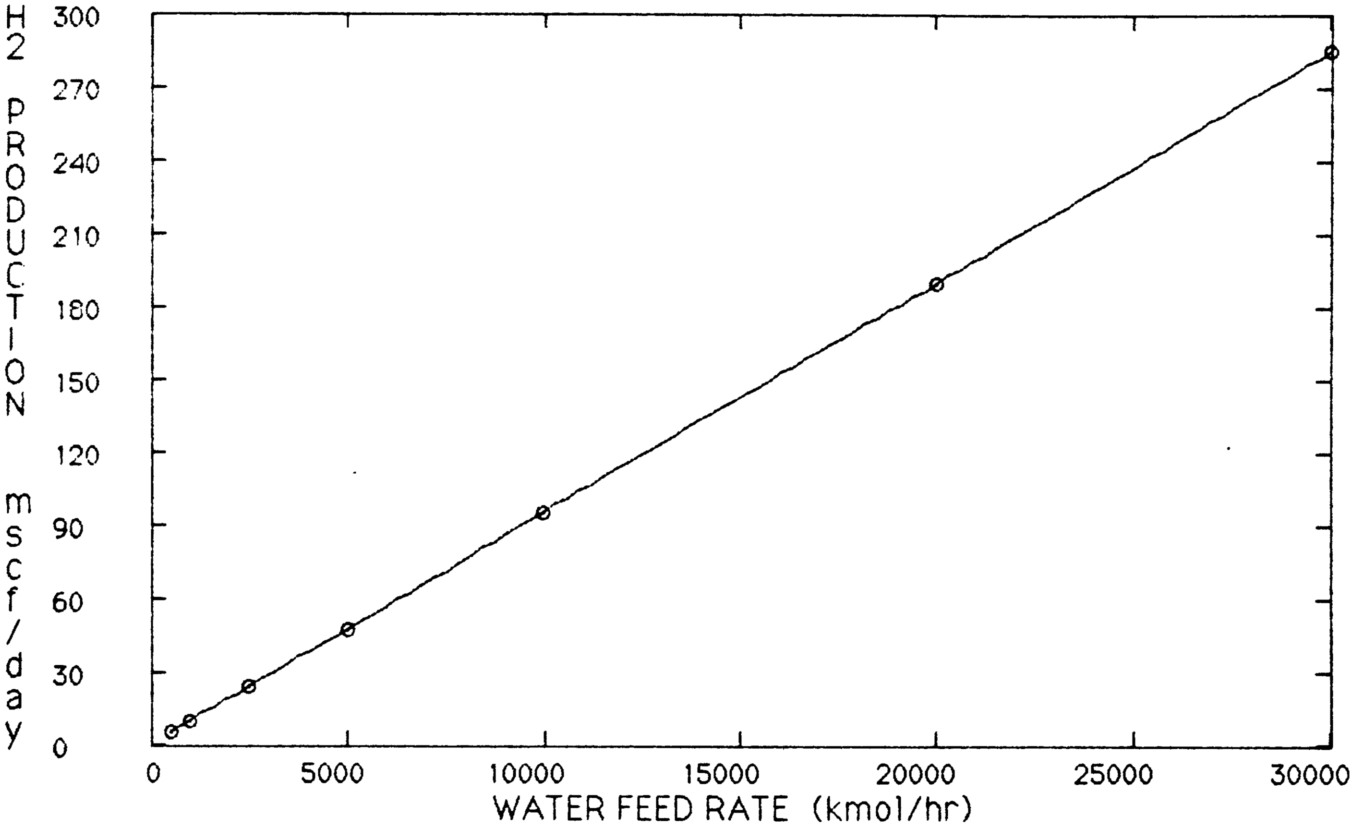


FIGURE 30: Daily hydrogen production rate from the electrolysis system versus the water feed flow rate

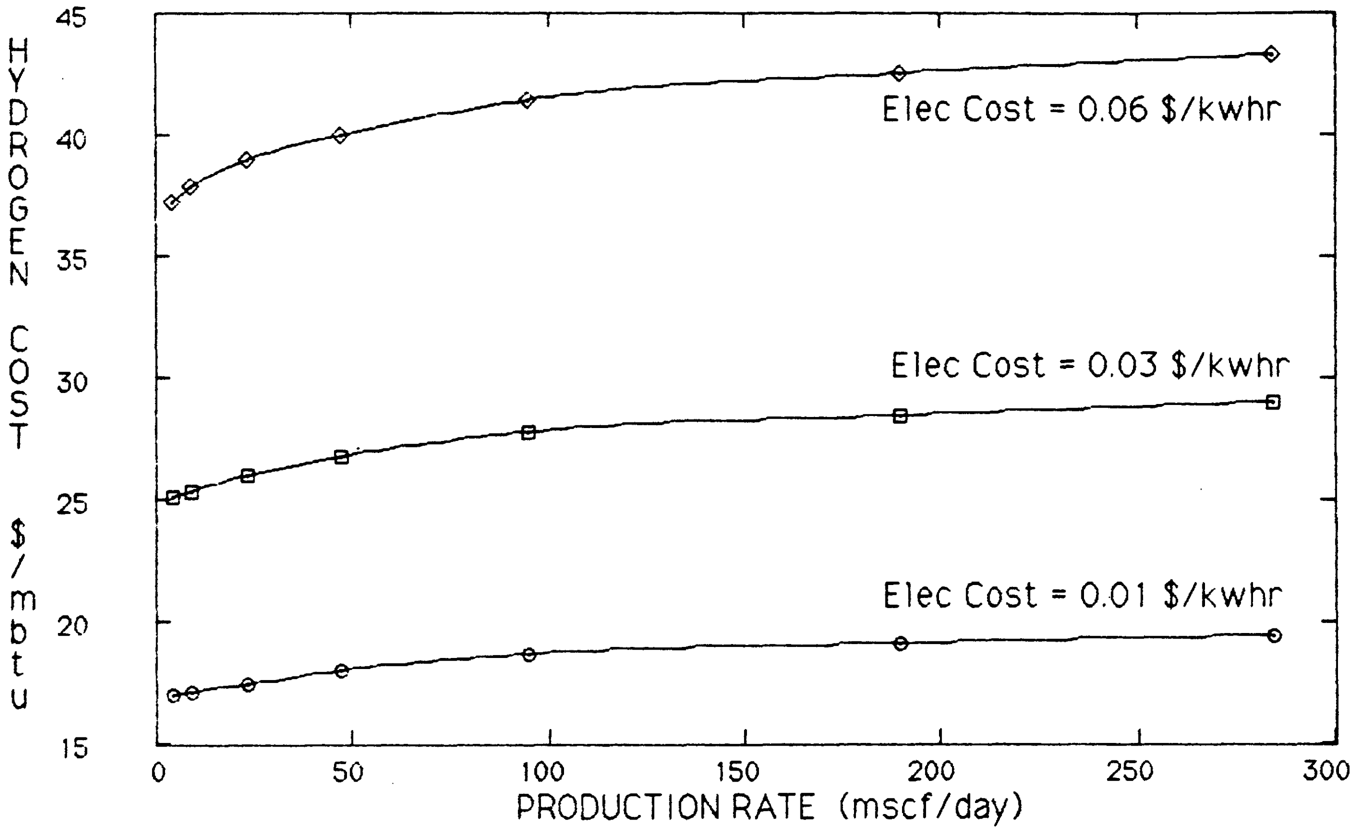


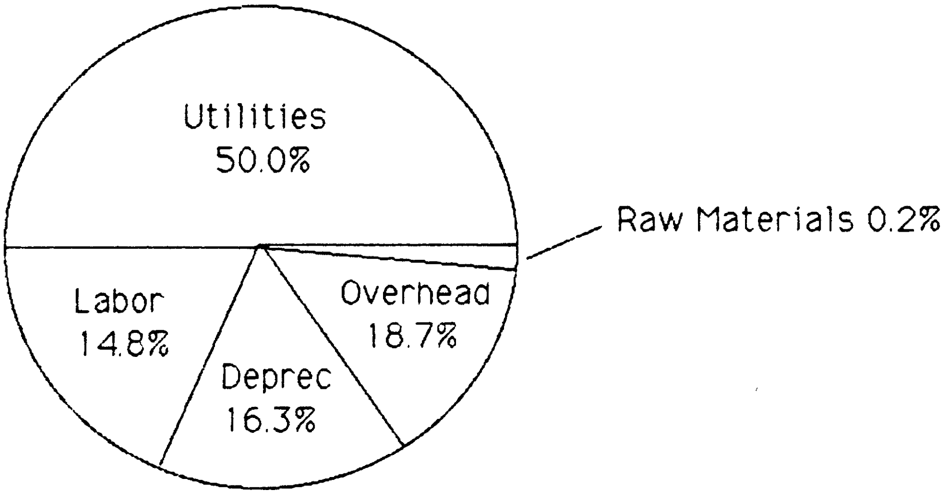
FIGURE 31: Cost of hydrogen produced by electrolysis versus the plant capacity for several electricity purchase costs

PLANT CAPACITY: 300 million scf per day

OPERATING PARAMETERS:
Water Feed Rate = 30,000 kmol/hr

OPERATING COST = $ 28.95 per million btu hydrogen

OPERATING COST BREAKDOWN:



CAPITAL COST SUMMARY:

Process Units	$ 1,179,678,000
Other Directs	447,250,000
Setting Labor	369,746,000
Contingency	583,823,000
Working Capital	289,498,000
Start up Cost	259,989,000
TOTAL:	$ 3,129,984,000

FIGURE 32: Operating and capital cost breakdowns for a 300 mscf per day hydrogen plant using electrolysis

resulting operating cost is $28.95 - much higher than either of the other two processes. A large part of the operating cost is the utility bill (i.e. electricity). However, an unexpectedly large part of the cost is in labor, overhead and depreciation. These costs are all associated with the capital investment (e.g. high capital investment leads to high depreciation costs), and as seen at the bottom of Figure 32 the capital for this plant is huge. For a plant this size running only on electrolysis units, over $3 billion would be required, and over $1 billion of it would be spent on enough large electrolysis units to handle the capacity. These costs are far in excess of those from the previous processes.

PROCESS COMPARISONS

One of the advantages to using flowsheet simulation as a tool is the ability to easily compare alternatives and look for viable versus impossible processes. Figure 33 shows a comparison of steam reforming to partial oxidation based on plant capacity. Two partial oxidation curves are shown, each representing a different oxygen purchase cost. The dashed line represents reforming. Clearly, if the oxygen cost is high, steam reforming is much more cost effective than partial oxidation. However, if cheap oxygen is available, the partial oxidation process can become competitive. This figure shows that if the oxygen cost was

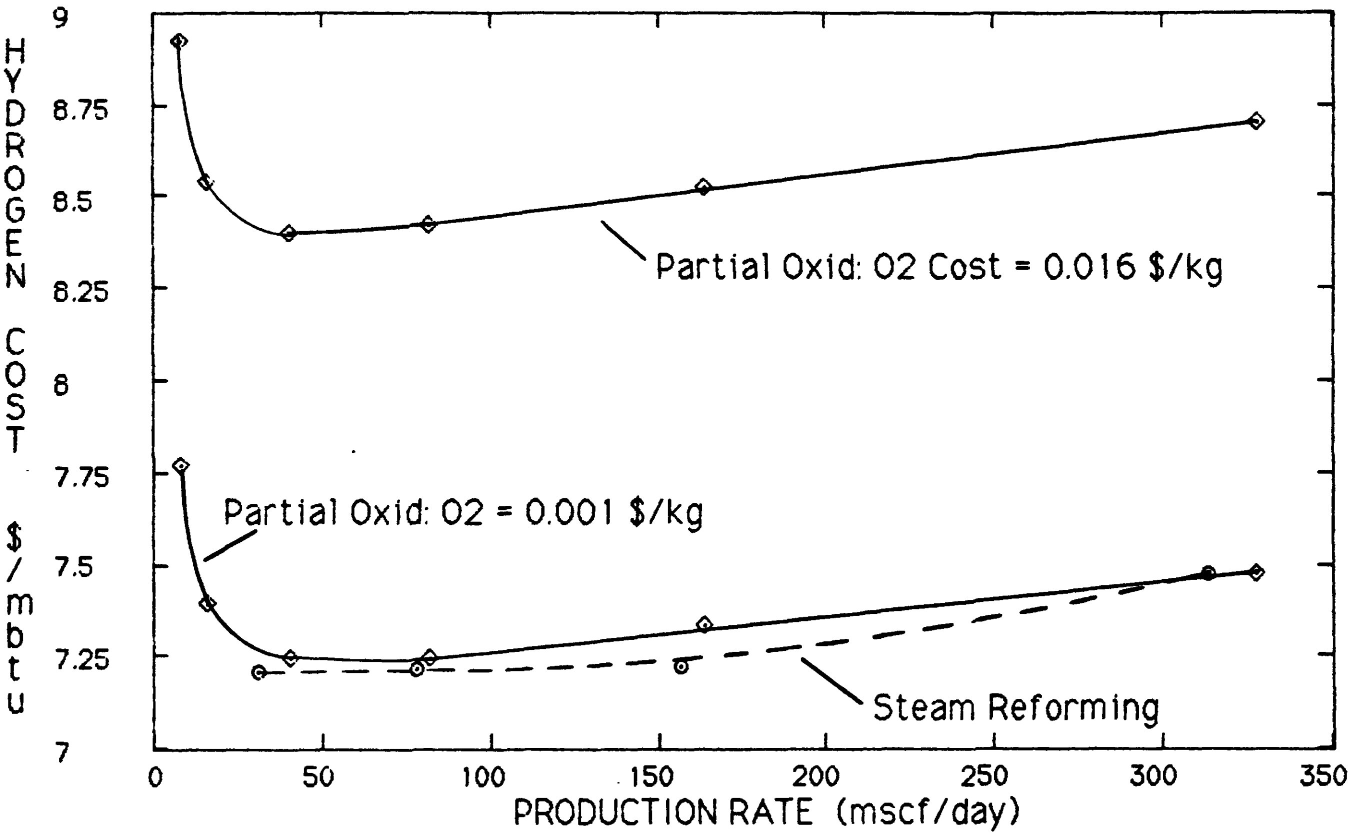


FIGURE 33: Cost of hydrogen versus production capacity for steam reforming and partial oxidation

about $0.001 per kilogram, partial oxidation and steam reforming would yield about the same cost hydrogen. So a decision of which process is better to pursue can be made based on the expected oxygen cost for the site.

Figure 34 shows a similar comparison of steam reforming and electrolysis. Even with relatively inexpensive electricity, electrolysis cannot compare to steam reforming at these production rates. The high capital cost of electrolysis combined with the electrical utility cost make electrolysis on this scale prohibitive. This suggests that in terms of hydrogen production on this scale, electrolysis is not a viable alternative.

Finally, Figure 35 provides a comparison of the operating and capital costs for a 300 mscf/day hydrogen plant for the three processes studied. As indicated, in terms of operating costs steam reforming is favored somewhat over partial oxidation and both are greatly favored over electrolysis. As for capital investment, the partial oxidation plant, using a less complex primary reactor, is least expensive. The steam reforming plant is somewhat more expensive, and the electrolysis plant is extremely expensive compared to the others.

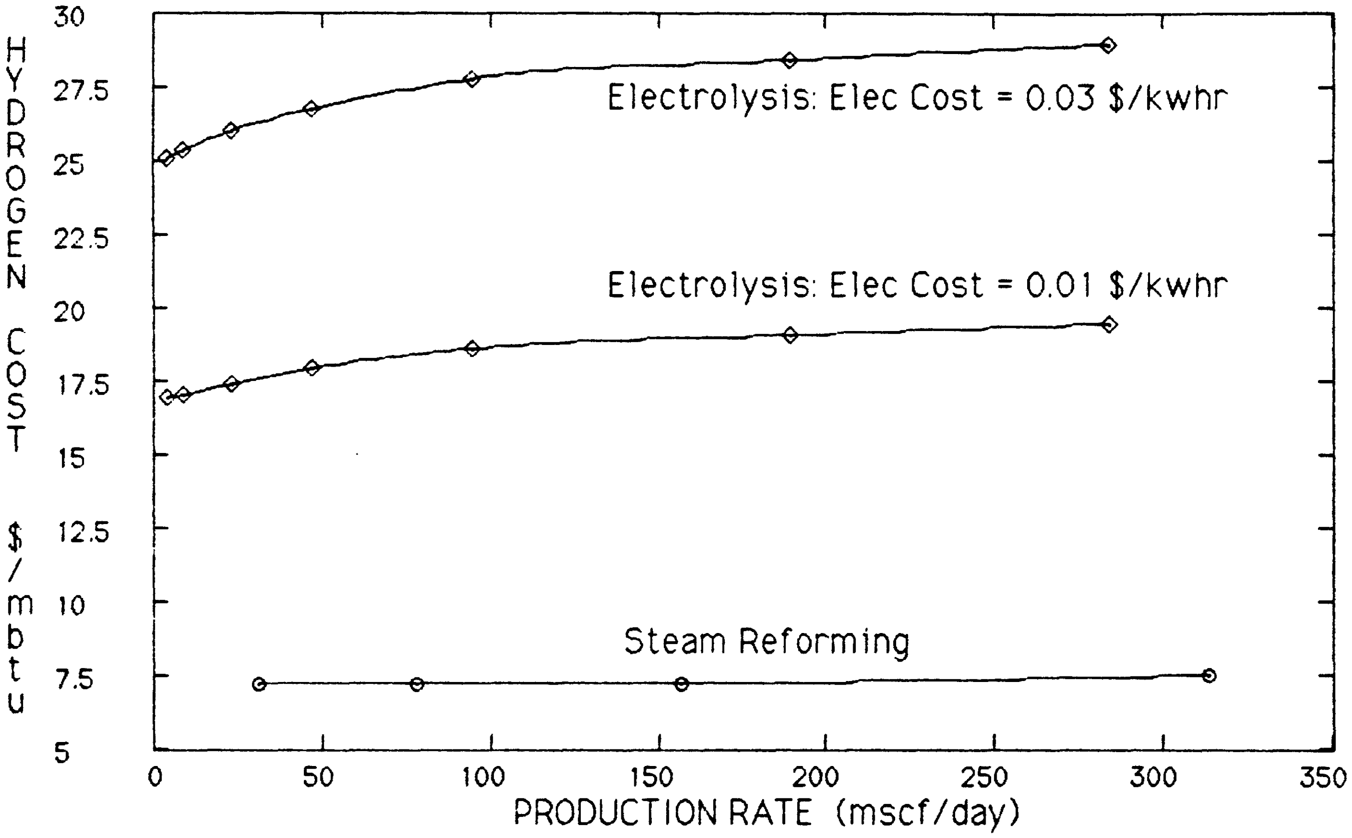


FIGURE 34: Cost of hydrogen versus production capacity for steam reforming and electrolysis

- OPERATING COST COMPARISON FOR 300 mscf/day PLANT:

Process	Hydrogen Cost ($/mbtu)
Steam Reforming	$ 7.43
Partial Oxidation	8.74
Electrolysis	28.95

- CAPITAL INVESTMENT COMPARISON FOR 300 mscf/day PLANT:

Process	Total Capital Investment
Steam Reforming	$ 332,316,000
Partial Oxidation	186,638,000
Electrolysis	3,129,984,000

FIGURE 35: Operating and capital cost comparison for the three hydrogen processes simulated

IV. CONCLUSIONS

Three different hydrogen production process have been simulated and analyzed. Two of them, steam reforming and partial oxidation, were similar enough for direct comparison of many of the operating parameters and results. The third, electrolysis, showed a completely different type of technology, yet through the simulations, it was possible to compare the ultimate cost performance of this system with the other two.

With the steam reforming and partial oxidation processes, it was demonstrated how the simulations could be used to set the primary reactor operating conditions so as to achieve the most cost effective product. This optimization not only helps to determine proper operating conditions given the process, but also the optimum cost results could be used during the design process to select the best process pathway to follow. In addition, the results from the simulations could be used to help guide research work. For example, in both cases, temperatures above 1200K yielded no advantage, so work need not be done on catalysts for higher temperatures.

The final comparison of steam reforming to partial oxidation showed that steam reforming is favored, primarily because pure oxygen is not used in the process. As had been expected, the oxygen needed in partial oxidation, unless very cheap, imposes a high operating cost on the process.

The electrolysis simulation showed that steam reforming is much more cost effective than electrolysis. This occurs even at low electricity cost, suggesting that the capital cost associated with electrolysis on the scale of 300 mscf/day is the prohibiting factor. Here again the results can guide research. The key need is not for cheaper electricity or more efficient electrical production. Instead, research should be concentrated on manufacturing a high capacity electrolysis cell with the same or better efficiency at a fraction of the capital investment.

This study has demonstrated the power of flowsheet simulation as a tool in technological development. By combining process and cost performance, several process alternatives, even based on different technologies, can be readily compared. This comparison aids in eliminating improbable processes early in development and deciding on which process is the most viable to pursue in the future. With a process selected, flowsheet simulation further helps in driving the research necessary to make the desired process possible and cost effective in the long run.

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APPENDIX:

ASPEN Input Files

LISTING 1

```
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;                      BY JOHN E. STRONG, JR.
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             BY MEANS OF STEAM REFORMING OF METHANE GAS."
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OUT-UNITS MET
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;
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   BLOCK COOL2     IN=HTSFTOUT       OUT=LTSFTIN
   BLOCK LTSHIFT   IN=LTSFTIN        OUT=LTSFTOUT
   BLOCK COOL3     IN=LTSFTOUT       OUT=SCRUBIN
   BLOCK SCRB-MIX     IN=SCRUBIN LMEA   OUT=SCRUBCOM
   BLOCK SCRB-SEP   IN=SCRUBCOM   OUT=HMEA SCRUBOUT
   BLOCK MEA-HEAT  IN=HMEA  OUT=HOTMEA
   BLOCK MEA-REC   IN=HOTMEA   OUT=RMEA CO2EXIT
   BLOCK HEAT1     IN=SCRUBOUT       OUT=HOTSCRUB
   BLOCK METHATOR   IN=HOTSCRUB   OUT=WET-PROD
   BLOCK H2O-SEP     IN=WET-PROD   OUT=H2OEXIT PRODUCT
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;          INPUT STREAM SPECIFICATIONS
;
STREAM FEED TEMP=500 PRES=20 NPHASE=1 PHASE=V MOLE-FLOW=10000.0
   MOLE-FRAC CH4 1.0
STREAM STEAM TEMP=550 PRES=20 NPHASE=1 PHASE=V MOLE-FLOW=40000.0
   MOLE-FRAC H2O 1.0
;
STREAM LMEA TEMP=320 PRES=20 NPHASE=1 PHASE=L MOLE-FLOW=50000.0
   MOLE-FRAC DEA 0.0684/ H2O 0.9316
;
;         BLOCK DATA
;
FORTRAN SET-INIT
   DEFINE XFM STREAM-VAR STREAM=FEED VARIABLE=MOLE-FLOW
   DEFINE XC1 CBLOCK-VAR CBLOCK=CHTS SENTENCE=SIZING-DATA &
     VARIABLE=CAP
   DEFINE XC2 CBLOCK-VAR CBLOCK=CLTS SENTENCE=SIZING-DATA &
     VARIABLE=CAP
   DEFINE XC3 CBLOCK-VAR CBLOCK=CMETH SENTENCE=SIZING-DATA &
     VARIABLE=CAP
F      XC1=XFM
F      XC2=XFM
F      XC3=XFM
   EXECUTE FIRST
;
BLOCK REFORMER RGIBBS
```

```
         NATOM=3 NREAC=2
   PROD  H2/ CO/ CO2/ CH4/ H2O
:   ATOMS           C     H     O
   ATOM  H2  1      0 /   2 /   0 /
         CO  1      1 /   0 /   1 /
         CO2 1      1 /   0 /   2 /
         CH4 1      1 /   4 /   0 /
         H2O 1      0 /   2 /   1
   STOIC 1 CH4 -1/ H2O -1/ CO 1/ H2 3
   STOIC 2 CO -1/ H2O -1/ CO2 1/ H2 1
   TAPP-SPEC 1 -15
   TAPP-SPEC 2 0
;
BLOCK COOL1 HEATER
   PARAM TEMP=670 PRES=0 NPHASE=1 PHASE=V
;
BLOCK HTSHIFT RGIBBS
   PARAM TEMP=670 PRES=-2 NPHASE=1 VAPOR=1 &
         NATOM=3 NREAC=2
   PROD H2/ CO/ CO2/ H2O/ CH4
:  ATOMS             C     H     O
   ATOM  H2   1      0 /   2 /   0 /
         CH4  1      1 /   4 /   0 /
         CO   1      1 /   0 /   1 /
         CO2  1      1 /   0 /   2 /
         H2O  1      0 /   2 /   1
   STOIC 1 CO -1/ H2O -1/ H2 1/ CO2 1
   TAPP-SPEC 1 10
   STOIC 2 CH4 -1/ H2O -1/ CO 1/ H2 3
   EXTENT-SPEC 2 0.0
;
BLOCK COOL2 HEATER
   PARAM TEMP=470 PRES=0 NPHASE=1 PHASE=V
;
BLOCK LTSHIFT RGIBBS
   PARAM TEMP=470 PRES=-2 NPHASE=1 VAPOR=1 &
         NATOM=3 NREAC=2
   PROD H2/ CO/ CO2/ H2O/ CH4
:  ATOMS             C     H     O
   ATOM   H2   1     0 /   2 /   0 /
          CH4  1     1 /   4 /   0 /
          CO   1     1 /   0 /   1 /
          CO2  1     1 /   0 /   2 /
          H2O  1     0 /   2 /   1
   STOIC 1 CO -1/ H2O -1/ H2 1/ CO2 1
   TAPP-SPEC 1 10
   STOIC 2 CH4 -1/ H2O -1/ CO 1/ H2 3
   EXTENT-SPEC 2 0.0
;
BLOCK COOL3 HEATER
   PARAM TEMP=320 PRES=0 NPHASE=1 PHASE=V
;
BLOCK SCRB-MIX HEATER
   PARAM TEMP=320 PRES=0
;
BLOCK SCRB-SEP SEP
   FRAC STREAM=HMEA COMPS=DEA CO2 H2O FRACS=1.0 1.0 0.5
   FLASH-SPECS SCRUBOUT NPHASE=1 PHASE=V
;
BLOCK MEA-HEAT HEATER
   PARAM TEMP=400 PRES=0 NPHASE=1 PHASE=V
;
BLOCK MEA-REC SEP
   FRAC STREAM=RMEA COMPS=DEA FRACS=1.0
;
```

```
   PARAM TEMP=580 PRES=0 NPHASE=1 PHASE=V
;
BLOCK METHATOR RSTOIC
   PARAM TEMP=600 PRES=-2 NPHASE=1 PHASE=V
   STOIC 1 MIXED CO -1/ H2 -3/ CH4 1/ H2O 1
   CONV 1 MIXED CO 1.0
;
BLOCK H2O-SEP SEP
   FRAC STREAM=H2OEXIT COMPS=H2O FRACS=1.0
;
;          COSTING SECTION
;
CBLOCK CHTS USER
   SIZING-DATA CAP=0.0
   COSTING-DATA NEQUIP=1
   USER-CORR REF-COST=100000 REF-CAP=5000 EXPON=0.5 &
     MIN-CAP=100 MAX-CAP=1.0E6
;
CBLOCK CLTS USER
   SIZING-DATA CAP=0.0
   COSTING-DATA NEQUIP=1
   USER-CORR REF-COST=100000 REF-CAP=5000 EXPON=0.5 &
     MIN-CAP=100 MAX-CAP=1.0E6
;
CBLOCK CMETH USER
   SIZING-DATA CAP=0.0
   COSTING-DATA NEQUIP=1
   USER-CORR REF-COST=50000 REF-CAP=5000 EXPON=0.5 &
     MIN-CAP=100 MAX-CAP=1.0E6
;
CBLOCK CSCRUB TRAY-TOWER
   SIZING-DATA DIAM=5<FT> NTRAY=10 PRES=5 TEMP=350
   COSTING-DATA TYPE=ABSORPTION NEQUIP=1
;
CBLOCK CKNOCK V-VESSEL
   SIZING-DATA DIAM=5<FT> TT-LENGTH=10<FT> TEMP=500 PRES=5
   COSTING-DATA NEQUIP=1
;
CBLOCK CMEA HEATX
   REFERENCE SHELL UTILITY=STM1
   REFERENCE TUBE BLOCK=MEA-HEAT
   SIZING-DATA U=350<BTU/HR-SQFT-R>
;
CBLOCK CCOOL1 HEATX
   REFERENCE SHELL UTILITY=COOL-H2O
   REFERENCE TUBE BLOCK=COOL1
   SIZING-DATA U=50<BTU/HR-SQFT-R>
;
CBLOCK CCOOL2 HEATX
   REFERENCE SHELL UTILITY=COOL-H2O
   REFERENCE TUBE BLOCK=COOL2
   SIZING-DATA U=50<BTU/HR-SQFT-R>
;
CBLOCK CCOOL3 HEATX
   REFERENCE SHELL UTILITY=COOL-H2O
   REFERENCE TUBE BLOCK=COOL3
   SIZING-DATA U=50<BTU/HR-SQFT-R>
;
CBLOCK CHEAT1 HEATX
   REFERENCE SHELL UTILITY=STM1
   REFERENCE TUBE BLOCK=HEAT1
   SIZING-DATA U=50<BTU/HR-SQFT-R>
;
FORTRAN REF-DUTY
   DEFINE XD1 BLOCK-VAR BLOCK=REFORMER SENTENCE=PARAM &
```

```
   DEFINE XD2 CBLOCK-VAR CBLOCK=CREF SENTENCE=SIZING-DATA &
     VARIABLE=DUTY
F      XD2=XD1
   EXECUTE AFTER REFORMER
;
CBLOCK CREF FURNACE
   SIZING-DATA DUTY=0.0
   COSTING-DATA TYPE=REFORMER PRES=8
   UTILITY GAS=FUEL-GAS
;
UTILITY STM1 STEAM
   SOURCE PURCHASED
   PROPERTIES SYSOP12
   PARAM COMPONENT=H2O TIN=700 TOUT=700 PRES=15
   COST PRICE=2.0E-3<$/LB>
;
UTILITY FUEL-GAS GAS
   SOURCE PURCHASED
   COST PRICE=0.01<$/KWHR>
;
UTILITY COOL-H2O WATER
   SOURCE PURCHASED
   PROPERTIES SYSOP12
   PARAM COMPONENT=H2O
   COST PRICE=1.2E-4<$/LB>
;
RAW-MATERIAL CH4-IN
   REFERENCE STREAM=FEED
   COST PRICE=0.05<$/LB>
;
RAW-MATERIAL STM-IN
   REFERENCE STREAM=STEAM
   COST PRICE=2.0E-3<$/LB>
;
UNIT REFORM
   CBLOCKS CREF CHTS CLTS CMETH CSCRUB CKNOCK CMEA CCOOL1 &
           CCOOL2 CCOOL3 CHEAT1
;
OPERATING-COST
   OPERATING-LABOR NOPER=2 RATE=10.00
   AVAILABILITY FACTOR=0.5
;
PROJECT-DATES
   START APRIL 1986
;
LABOR-COSTS
   WAGES RATE=20.0
   JOB-CONDITION LOCATION=MIT
;
COSTING-OPTIONS OPER-COST
;
SENSITIVITY RESULTS
   DESCRIPTION 'STEAM REFORMING RESULTS'
   DEFINE S1 MOLE-FLOW STREAM=PRODUCT COMPONENT=H2
   DEFINE S2 MOLE-FLOW STREAM=PRODUCT COMPONENT=CH4
   DEFINE S3 OPER-COST-VAR SENTENCE=RESULTS &
     VARIABLE=NET-OP-COST
   DEFINE S4 OPER-COST-VAR SENTENCE=AVAILABILITY &
     VARIABLE=FACTOR
;      CALCULATE PURITY:
F      S5=S1/(S1+S2)
;      CALCULATE VOLUME PER DAY PRODUCED (SCF):
F      S6=S1*1000.0*24.0*S4*0.791/1E6
;      CALCULATE COST PER MILLION BTU:
F      S7=S3/(S1*1000.0*24.0*365.0*S4*271.3/1E6)
```

```
    TABULATE 1 65 COL-LABEL='% H2' 'IN' 'PRODUCT' 'STREAM'
    TABULATE 2 66 COL-LABEL='PRODUCT' 'RATE' 'OF H2' &
      UNIT-LABEL='MSCF/DAY'
    TABULATE 3 67 COL-LABEL='PRODUCT' 'COST' UNIT-LABEL='$/MBTU'
    VARY STREAM-VAR STREAM=STEAM VARIABLE=MOLE-FLOW
    RANGE LIST=20000 25000 30000 35000 40000 45000 50000


$
```

LISTING 2

```
;
;          HYDROGEN MANUFACTURE -- PARTIAL OXIDATION
;                      BY JOHN E. STRONG, JR.
;
TITLE 'HYDROGEN MANUFACTURE BY PARTIAL OXIDATION OF HYDROCARBONS'
DESCRIPTION "THIS FLOWSHEET MODELS THE MANUFACTURE OF HYDROGEN
             BY MEANS OF PARTIAL OXIDATION OF HYDROCARBONS:
             FEEDS CAN INCLUDE -
                     METHANE = CH4
                     NAPHTHA = CH2.2
                     COAL    = CH0.8"
IN-UNITS MET
OUT-UNITS MET
SYS-OPTIONS INTERPRET=0
RUN-CONTROL MAX-TIME=500
;
;          COMPONENTS
;
COMPONENTS H2 H2/CO2 CO2/CO CO/H2O H2O/CH4 CH4/O2 O2/
     DEA C4H11NO2-1
PROPERTIES SYSOP3
;
;          FLOWSHEET DATA
;
FLOWSHEET
   BLOCK OXIDIZER  IN=FEED STEAM O2FEED OUT=OXOUT
   BLOCK COOL1     IN=OXOUT         OUT=HTSFTIN
   BLOCK HTSHIFT   IN=HTSFTIN        OUT=HTSFTOUT
   BLOCK COOL2     IN=HTSFTOUT       OUT=LTSFTIN
   BLOCK LTSHIFT   IN=LTSFTIN        OUT=LTSFTOUT
   BLOCK COOL3     IN=LTSFTOUT       OUT=SCRUBIN
   BLOCK SCRB-MIX     IN=SCRUBIN LMEA   OUT=SCRUBCOM
   BLOCK SCRB-SEP   IN=SCRUBCOM   OUT=HMEA SCRUBOUT
   BLOCK MEA-HEAT   IN=HMEA    OUT=HOTMEA
   BLOCK MEA-REC   IN=HOTMEA   OUT=RMEA CO2EXIT
   BLOCK HEAT1     IN=SCRUBOUT       OUT=HOTSCRUB
   BLOCK METHATOR   IN=HOTSCRUB   OUT=WET-PROD
   BLOCK H2O-SEP     IN=WET-PROD   OUT=H2OEXIT PRODUCT
;
;          INPUT STREAM SPECIFICATIONS
;
STREAM FEED TEMP=500 PRES=20 NPHASE=1 PHASE=V MOLE-FLOW=10000.0
   MOLE-FRAC CH4 1.0
STREAM STEAM TEMP=550 PRES=20 NPHASE=1 PHASE=V MOLE-FLOW=10000
   MOLE-FRAC H2O 1.0
STREAM O2FEED TEMP=500 PRES=20 NPHASE=1 PHASE=V MOLE-FLOW=10000
   MOLE-FRAC O2 1.0
;
STREAM LMEA TEMP=320 PRES=20 NPHASE=1 PHASE=L MOLE-FLOW=50000.0
   MOLE-FRAC DEA 0.0684/ H2O 0.9316
;
;         BLOCK DATA
;
BLOCK OXIDIZER RGIBBS
   PARAM PRES=20 TEMP=1000 NPHASE=1 VAPOR=1 &
         NATOM=3
   PROD H2/ CO/ CO2/ CH4/ H2O/ O2
;   ATOMS          C     H     O
   ATOM  H2  1     0 /   2 /   0 /
```

```
         CO2 1      1 /   0 /   2 /
         CH4 1      1 /   4 /   0 /
         H2O 1      0 /   2 /   1 /
         O2  1      0 /   0 /   2
;
BLOCK COOL1 HEATER
   PARAM TEMP=670 PRES=0 NPHASE=1 PHASE=V
;
BLOCK HTSHIFT RGIBBS
   PARAM TEMP=670 PRES=-2 NPHASE=1 VAPOR=1 &
         NATOM=3 NREAC=3
   PROD H2/ CO/ CO2/ H2O/ CH4/ O2
;    ATOMS             C      H      O
   ATOM  H2   1      0 /    2 /    0 /
         CH4  1      1 /    4 /    0 /
         CO   1      1 /    0 /    1 /
         CO2  1      1 /    0 /    2 /
         H2O  1      0 /    2 /    1 /
         O2   1      0 /    0 /    2
   STOIC 1 CO -1/ H2O -1/ H2 1/ CO2 1
   TAPP-SPEC 1 14
   STOIC 2 CH4 -1/ H2O -1/ CO 1/ H2 3
   EXTENT-SPEC 2 0.0
   STOIC 3 H2 -2/ O2 -1/ H2O 2
   EXTENT-SPEC 3 0.0
;
BLOCK COOL2 HEATER
   PARAM TEMP=470 PRES=0 NPHASE=1 PHASE=V
;
BLOCK LTSHIFT RGIBBS
   PARAM TEMP=470 PRES=-2 NPHASE=1 VAPOR=1 &
         NATOM=3 NREAC=3
   PROD H2/ CO/ CO2/ H2O/ CH4/ O2
;  ATOMS                C     H      O
   ATOM   H2   1     0 /   2 /    0 /
          CH4  1     1 /   4 /    0 /
          CO   1     1 /   0 /    1 /
          CO2  1     1 /   0 /    2 /
          H2O  1     0 /   2 /    1 /
          O2   1     0 /   0 /    2
   STOIC 1 CO -1/ H2O -1/ H2 1/ CO2 1
   TAPP-SPEC 1 14
   STOIC 2 CH4 -1/ H2O -1/ CO 1/ H2 3
   EXTENT-SPEC 2 0.0
   STOIC 3 H2 -2/ O2 -1/ H2O 2
   EXTENT-SPEC 3 0.0
;
BLOCK COOL3 HEATER
   PARAM TEMP=320 PRES=0 NPHASE=1 PHASE=V
;
BLOCK SCRB-MIX HEATER
   PARAM TEMP=320 PRES=0
;
BLOCK SCRB-SEP SEP
   FRAC STREAM=HMEA COMPS=DEA CO2 H2O O2 FRACS=1.0 1.0 0.5 1.0
   FLASH-SPECS SCRUBOUT NPHASE=1 PHASE=V
;
BLOCK MEA-HEAT HEATER
   PARAM TEMP=400 PRES=0 NPHASE=1 PHASE=V
;
BLOCK MEA-REC SEP
   FRAC STREAM=RMEA COMPS=DEA FRACS=1.0
;
BLOCK HEAT1 HEATER
   PARAM TEMP=580 PRES=0 NPHASE=1 PHASE=V
```

```
BLOCK METHATOR RSTOIC
   PARAM TEMP=600 PRES=-2 NPHASE=1 PHASE=V
   STOIC 1 MIXED CO -1/ H2 -3/ CH4 1/ H2O 1
   CONV 1 MIXED CO 1.0
;
BLOCK H2O-SEP SEP
   FRAC STREAM=H2OEXIT COMPS=H2O FRACS=1.0
;
;          COSTING SECTION
;
CBLOCK COXID USER
   USER-COST PURCH-COST=300000
   COSTING-DATA NEQUIP=1
;
CBLOCK CHTS USER
   USER-COST PURCH-COST=200000
   COSTING-DATA NEQUIP=1
;
CBLOCK CLTS USER
   USER-COST PURCH-COST=200000
   COSTING-DATA NEQUIP=1
;
CBLOCK CMETH USER
   USER-COST PURCH-COST=100000
   COSTING-DATA NEQUIP=1
;
CBLOCK CSCRUB TRAY-TOWER
   SIZING-DATA DIAM=5<FT> NTRAY=10 PRES=5 TEMP=350
   COSTING-DATA TYPE=ABSORPTION NEQUIP=1
;
CBLOCK CKNOCK V-VESSEL
   SIZING-DATA DIAM=5<FT> TT-LENGTH=10<FT> TEMP=500 PRES=5
   COSTING-DATA NEQUIP=1
;
CBLOCK CMEA HEATX
   REFERENCE SHELL UTILITY=STM1
   REFERENCE TUBE BLOCK=MEA-HEAT
   SIZING-DATA U=350<BTU/HR-SQFT-R>
;
CBLOCK CCOOL1 HEATX
   REFERENCE SHELL UTILITY=COOL-H2O
   REFERENCE TUBE BLOCK=COOL1
   SIZING-DATA U=50<BTU/HR-SQFT-R>
;
CBLOCK CCOOL2 HEATX
   REFERENCE SHELL UTILITY=COOL-H2O
   REFERENCE TUBE BLOCK=COOL2
   SIZING-DATA U=50<BTU/HR-SQFT-R>
;
CBLOCK CCOOL3 HEATX
   REFERENCE SHELL UTILITY=COOL-H2O
   REFERENCE TUBE BLOCK=COOL3
   SIZING-DATA U=50<BTU/HR-SQFT-R>
;
CBLOCK CHEAT1 HEATX
   REFERENCE SHELL UTILITY=STM1
   REFERENCE TUBE BLOCK=HEAT1
   SIZING-DATA U=50<BTU/HR-SQFT-R>
;
FORTRAN OX-DUTY
   DEFINE XD1 BLOCK-VAR BLOCK=OXIDIZER SENTENCE=PARAM &
     VARIABLE=QCALC
   DEFINE XD2 CBLOCK-VAR CBLOCK=COXID SENTENCE=SIZING-DATA &
     VARIABLE=DUTY
F      XD3=XD1
```

```
F      XO1=XO2
   EXECUTE AFTER OXIDIZER
;
CBLOCK COXID FURNACE
   SIZING-DATA DUTY=0
   COSTING-DATA TYPE=PROCESS PRES=8
   UTILITY GAS=FUEL-GAS
;
UTILITY STM1 STEAM
   SOURCE PURCHASED
   PROPERTIES SYSOP12
   PARAM COMPONENT=H2O TIN=700 TOUT=700 PRES=15
   COST PRICE=2.0E-3<$/LB>
;
UTILITY FUEL-GAS GAS
   SOURCE PURCHASED
   COST PRICE=0.01<$/KWHR>
;
UTILITY COOL-H2O WATER
   SOURCE PURCHASED
   PROPERTIES SYSOP12
   PARAM COMPONENT=H2O
   COST PRICE=1.2E-4<$/LB>
;
RAW-MATERIAL CH4-IN
   REFERENCE STREAM=FEED
   COST PRICE=0.05<$/LB>
;
RAW-MATERIAL STM-IN
   REFERENCE STREAM=STEAM
   COST PRICE=2.0E-3<$/LB>
;
RAW-MATERIAL O2-IN
   REFERENCE STREAM=O2FEED
   COST PRICE=0.0075<$/LB>
;
UNIT REFORM
   CBLOCKS COXID CHTS CLTS CMETH CSCRUB CKNOCK CMEA CCOOL1 &
           CCOOL2 CCOOL3 CHEAT1
;
OPERATING-COST
   OPERATING-LABOR NOPER=2 RATE=10.00
   AVAILABILITY FACTOR=0.5
;
PROJECT-DATES
   START MAY 1986
;
LABOR-COSTS
   WAGES RATE=20.0
   JOB-CONDITION LOCATION=MIT
;
COSTING-OPTIONS OPER-COST
;
SENSITIVITY RESULTS
   DESCRIPTION 'PARTIAL OXIDATION RESULTS'
   DEFINE S1 MOLE-FLOW STREAM=PRODUCT COMPONENT=H2
   DEFINE S2 MOLE-FLOW STREAM=PRODUCT COMPONENT=CH4
   DEFINE S3 OPER-COST-VAR SENTENCE=RESULTS &
     VARIABLE=NET-OP-COST
   DEFINE S4 OPER-COST-VAR SENTENCE=AVAILABILITY &
     VARIABLE=FACTOR
F      IF(S1.EQ.0.0) S1=1.0
F      IF(S2.EQ.0.0) S2=1.0
;      CALCULATE PURITY:
F      S5=S1/(S1+S2)
```

```
F      S6=S1*1000.0*24.0*S4*0.791/1E6
;      CALCULATE COST PER MILLION BTU:
F      S7=S3/(S1*1000.0*24.0*365.0*S4*271.3/1E6)
;
   TABULATE 1 S5 COL-LABEL='% H2' 'IN' 'PRODUCT' 'STREAM'
   TABULATE 2 S6 COL-LABEL='PRODUCT' 'RATE' 'OF H2' &
     UNIT-LABEL='MSCF/DAY'
   TABULATE 3 S7 COL-LABEL='PRODUCT' 'COST' UNIT-LABEL='$/MBTU'
   VARY STREAM-VAR STREAM=O2FEED VARIABLE=MOLE-FLOW
   RANGE LIST=5000 10000 15000
   VARY BLOCK-VAR BLOCK=OXIDIZER SENTENCE=PARAM VARIABLE=PRES
   RANGE LIST=10 15 20 25 30
;

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```

LISTING 3

```
;
;          HYDROGEN MANUFACTURE -- ELECTROLYSIS
;                      BY JOHN E. STRONG, JR.
;
TITLE 'HYDROGEN MANUFACTURE BY ELECTROLYSIS OF WATER'
DESCRIPTION "THIS FLOWSHEET MODELS THE MANUFACTURE OF HYDROGEN
             BY MEANS OF ELECTROLYSIS OF WATER"
IN-UNITS MET
OUT-UNITS MET
SYS-OPTIONS INTERPRET=0
;
;          COMPONENTS
;
COMPONENTS H2 H2/O2 O2/H2O H2O
PROPERTIES SYSOP3
;
;          FLOWSHEET DATA
;
FLOWSHEET
   BLOCK CELL    IN=FEED    OUT=GASES
   BLOCK CELLSEP  IN=GASES  OUT=H2UP O2UP
   BLOCK H2KNOCK   IN=H2UP  OUT=PRODUCT
   BLOCK O2KNOCK   IN=O2UP  OUT=O2EXIT
;
;          INPUT STREAM SPECIFICATIONS
;
STREAM FEED TEMP=340 PRES=1 NPHASE=1 PHASE=L MOLE-FLOW=30000
   MOLE-FRAC H2O 1.0
;
;          BLOCK DATA
;
BLOCK CELL RSTOIC
   PARAM TEMP=340 PRES=1
   STOIC 1 MIXED H2O -1/ H2 1/ O2 0.5
   CONV 1 MIXED H2O 1.0
;
BLOCK CELLSEP SEP
   FRAC STREAM=H2UP COMPS=H2 FRACS=1.0
;
BLOCK H2KNOCK MIXER
;
BLOCK O2KNOCK MIXER
;
;          COSTING SECTION
;
FORTRAN COST-SET
   DEFINE XF STREAM-VAR STREAM=FEED VARIABLE=MOLE-FLOW
   DEFINE XC1 CBLOCK-VAR CBLOCK=CCELL SENTENCE=USER-COST &
     VARIABLE=PURCH-COST
   DEFINE XC2 CBLOCK-VAR CBLOCK=CCELL SENTENCE=UTILITY &
     VARIABLE=ELEC-RATE
;
F      XC1=20000.0*XF
F      XC2=93.47*XF
;
   EXECUTE BEFORE CCELL
;
CBLOCK CCELL USER
   COSTING-DATA NEQUIP=1
```

```
   UTILITY ELEC=POWER ELEC-RATE=0.0
;
UNIT ELECTOLYSIS
   CBLOCKS CCELL
;
UTILITY POWER ELECTRICITY
   SOURCE PURCHASED
   COST PRICE=0.03
;
RAW-MATERIAL H2O-IN
   REFERENCE STREAM=FEED
   COST PRICE=2.3E-4<$/LB>
;
OPERATING-COST
   AVAILABILITY FACTOR=0.5
   OPERATING-LABOR NOPER=1 RATE=10.00
;
PROJECT-DATES
   START MAY 1986
;
LABOR-COSTS
   WAGES RATE=20.00
   JOB-CONDITION LOCATION=MIT
;
COSTING-OPTIONS OPER-COST
;
SENSITIVITY RESULTS
   DESCRIPTION 'ELECTROLYSIS RESULTS'
   DEFINE S1 MOLE-FLOW STREAM=PRODUCT COMPONENT=H2
   DEFINE S3 OPER-COST-VAR SENTENCE=RESULTS &
     VARIABLE=NET-OP-COST
   DEFINE S4 OPER-COST-VAR SENTENCE=AVAILABILITY &
     VARIABLE=FACTOR
;     CALCULATE VOLUME PER DAY PRODUCED (MSCF):
F     R1=S1*1000.0*24.0*S4*0.791/1E6
;     CALCULATE COST PER MILLION BTU:
F     R2=S3/(S1*1000.0*24.0*365.0*S4*271.3/1E6)
;
   TABULATE 1 R1 COL-LABEL='PRODUCT' 'RATE' 'OF H2' &
     UNIT-LABEL='MSCF/DAY'
   TABULATE 2 R2 COL-LABEL='PRODUCT' 'COST' UNIT-LABEL='$/MBTU'
;
   VARY UTILITY-VAR UTILITY=POWER SENTENCE=COST VARIABLE=PRICE
   RANGE LIST=0.01 0.03 0.06
   VARY STREAM-VAR STREAM=FEED VARIABLE=MOLE-FLOW
   RANGE LIST=500 1000 2500 5000 10000 20000 30000


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```