Optimized Flow Sheet for a Reference Commercial-Scale Nuclear-Driven High-Temperature Electrolysis Hydrogen Production Plant

M. G. McKellar

J. E. O'Brien

E. A. Harvego

J. S. Herring

November 2007



The INL is a U.S. Department of Energy National Laboratory operated by Battelle Energy Alliance

Optimized Flow Sheet for a Reference Commercial-Scale Nuclear-Driven High-Temperature Electrolysis Hydrogen Production Plant

M. G. McKellar J. E. O'Brien E. A. Harvego J. S. Herring

November 2007

Idaho National Laboratory Idaho Falls, Idaho 83415

Prepared for the
U.S. Department of Energy
Office of Nuclear Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

DISCLAIMER

This information was prepared as an account of work sponsored by an agency of the U.S. Government. Neither the U.S. Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. References herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the U.S. Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the U.S. Government or any agency thereof.



ABSTRACT

This report presents results from the development and optimization of a reference commercialscale high-temperature electrolysis (HTE) plant for hydrogen production. The reference plant design is driven by a high-temperature helium-cooled reactor coupled to a direct Brayton power cycle. The reference design reactor power is 600 MWt, with a primary system pressure of 7.0 MPa, and reactor inlet and outlet fluid temperatures of 540° C and 900°C, respectively. The electrolysis unit used to produce hydrogen consists of 4.176×10^6 cells with a per-cell active area of 225 cm². A nominal cell area-specific resistance, ASR, value of 0.4 Ohm·cm² with a current density of 0.25 A/cm² was used, and isothermal boundary conditions were assumed. The optimized design for the reference hydrogen production plant operates at a system pressure of 5.0 MPa, and utilizes an air-sweep system to remove the excess oxygen that is evolved on the anode side of the electrolyzer. The inlet air for the air-sweep system is compressed to the system operating pressure of 5.0 MPa in a four-stage compressor with intercooling. The overall system thermal-to-hydrogen production efficiency (based on the low heating value of the produced hydrogen) is 49.07% at a hydrogen production rate of 2.45 kg/s with the high-temperature helium-cooled reactor concept. The information presented in this report is intended to establish an optimized design for the reference nuclear-driven HTE hydrogen production plant so that parameters can be compared with other hydrogen production methods and power cycles to evaluate relative performance characteristics and plant economics.

TABLE OF CONTENTS

ABS	STRACT	ii
TAI	BLE OF CONTENTS	iii
FIG	URES	iv
1.	INTRODUCTION	1
2.	SELECTION OF POWER CYCLE	1
2.	.1. Direct Helium Recuperated Brayton Cycle	2
3.	SELECTION OF THE REFERENCE HTE PROCESS	3
4.	COUPLING OF THE HTE PLANT AND REACTOR POWER CYCLE	4
5.	ELECTROLYZER MODEL	6
6.	OPTIMIZATION OF REFERENCE DESIGN	8
7.	REFERENCE DESIGN CONDITIONS	9
8.	CONCLUSIONS	16
9.	REFERENCES	17

FIGURES

Figure 1.	UniSim process flow diagram for helium recuperated direct Brayton cycle	3
Figure 2.	Process flow diagram for helium-cooled reactor/direct Brayton/HTE system with air sweep.	5
Figure 3.	Process flow diagram of electrolyzer model.	6
Figure 4.	Temperature profile plot of Brayton cycle recuperator.	13
Figure 5.	Temperature profile of Intermediate Heat Exchanger.	13
Figure 6.	Temperature profile of Electrolysis Heat Recuperator.	14
Figure 7.	Overall hydrogen product efficiency as a function of current density for an ASR of 0.4, isothermal boundary conditions, and constant steam utilization	15
Figure 8.	Overall hydrogen production efficiency as a function of steam utilization for an ASR of 0.4, adiabatic boundary conditions, and constant process and air sweep flows	15

TABLES

Table 1.	Electrolysis fluid stream conditions and flow rates.	7
Table 2.	Mole fraction composition data for electrolysis unit.	7
Table 3.	Isothermal electrolysis reaction (88.89% water conversion).	7
Table 4.	Isothermal flow and reaction balance (88.89% water conversion)	7
Table 5.	Stream fluid conditions and flow rates for reference plant design.	10
Table 6.	Mole fraction composition data for reference plant design	11
Table 7.	Component heat rates and electrolysis power for reference design.	12
Table 8.	Heat exchanger design parameters for reference plant design	12
Table 9.	Turbine design parameters for reference plant design.	12
Table 10.	Compressor design parameters for reference plant design.	12
Table 11.	Pump design parameters for reference plant design.	12

1. INTRODUCTION

This report presents results from the development and optimization of a reference commercialscale high-temperature electrolysis (HTE) plant for hydrogen production. The primary advantage of high temperature electrolysis over conventional electrolysis, which is a well established technology, is that considerably higher overall efficiencies can be achieved. The improved performance of HTE versus conventional low-temperature (alkaline or PEM) electrolysis is due to both the improved power-cycle efficiencies and electrolyzer efficiencies associated with high-temperature operation. Higher reactor outlet temperatures yield higher power cycle efficiencies in accordance with the Carnot principle. For example, power conversion thermal efficiencies in excess of 50% can be achieved with the high-temperature gascooled reactor coupled to the direct Brayton cycle [1]. The electrolyzer itself benefits from hightemperature operation for reasons related to both thermodynamics and kinetics. From thermodynamics, the electrical energy requirement for water or steam electrolysis decreases with increasing temperature, while the thermal energy requirement increases. Consequently, at higher temperatures, a larger fraction of the total electrolysis energy input can be supplied in the form of heat, increasing the overall process efficiency. In terms of kinetics, activation and ohmic electrochemical overpotentials also decrease dramatically with temperature.

UniSim process analysis software was used to evaluate the performance of the commercial-scale hydrogen production plant coupled to a high temperature helium cooled reactor. UniSim software is a derivative of the HYSYS process analysis software. UniSim inherently ensures mass and energy balances across all components and it includes thermodynamic data for all chemical species. The work described in this report establishes the optimized design based on analyses of process flow diagrams that include realistic representations of the reactor power source coupled to the Brayton power cycle and integrated with the high-temperature electrolysis process loops. As with previous HTE system analyses performed at the INL, a custom electrolyzer model was incorporated into the overall process flow sheet. This electrolyzer model allows for the determination of the average Nernst potential, cell operating voltage, gas outlet temperatures, and electrolyzer efficiency for any specified inlet steam, hydrogen, and sweep-gas flow rates, current density, cell active area, and external heat loss or gain. The electrolyzer model has been validated by comparison with results obtained from a fully 3-D computational fluid dynamics model and by comparison with experimental results. These comparisons may be found in Reference [3].

2. SELECTION OF POWER CYCLE

The selection of the reactor power cycle was based on previous parametric studies performed at the INL [2, 4]. In these previous studies, three advanced reactor – power cycle combinations were analyzed, including: a high-temperature helium-cooled reactor coupled to a direct helium recuperated Brayton cycle, a supercritical CO₂-cooled reactor coupled to a direct supercritical CO₂ recompression cycle, and a sodium-cooled fast reactor coupled to a tertiary steam Rankine cycle.

The three reactor power cycles evaluated were based on advanced reactor concepts capable of operating with reactor outlet temperatures in the range of 550°C to 900°C. These high temperatures result in higher power cycle efficiencies (33 to 55%) for these advanced reactor concepts than can be achieved with current generation light water reactors (30 to 35%). In addition, the high temperature process heat available from these advanced high temperature reactors can further enhance hydrogen production efficiencies when the reactor is directly coupled to a HTE hydrogen production plant.

The results of these studies showed that a high-temperature gas-cooled reactor directly coupled to a helium-recuperated Brayton cycle produced higher overall thermal-to-hydrogen production efficiencies (in the range of 45 - 50% efficiency) when compared to the supercritical CO2-cooled reactor utilizing a direct recompression power cycle (42 - 44% hydrogen production efficiency) and a sodium-cooled reactor utilizing an indirect Rankine cycle (33 - 34% hydrogen production efficiency).

Based on these results, a helium-cooled high-temperature gas-cooled reactor coupled to a direct helium recuperated Brayton power cycle was selected as the reference power source. This power system is described in more detail below.

2.1. Direct Helium Recuperated Brayton Cycle

A process flow diagram for the high-temperature helium-cooled reactor coupled to the direct helium recuperated Brayton cycle is presented in **Figure 1**. This UniSim power-cycle model was initially described in [4]. The primary helium coolant exits the reactor at 900°C. This helium flow is split at T1, with more than 85% of the flow directed toward the power cycle and the remainder directed to the intermediate heat exchanger to provide process heat to the HTE loop. Within the power-cycle loop, helium flows through the power turbine where the gas is expanded to produce electric power. The helium, at a reduced pressure and temperature, then passes through a recuperator and precooler where it is further cooled before entering the low-pressure compressor. To improve compression efficiencies, the helium is again cooled in an intercooler heat exchanger before entering the high-pressure compressor. The helium exits the high-pressure compressor at a pressure that is slightly higher than the reactor operating pressure of 7 MPa. The coolant then circulates back through the recuperator where the recovered heat raises its temperature to the reactor inlet temperature of 540°C, completing the cycle.

Process heat for the HTE hydrogen production plant is provided by splitting the reactor coolant outlet flow into two streams, and allowing a fraction (typically less than 15%) of the flow to pass through an intermediate heat exchanger where heat is extracted for use in the hydrogen production process. The cooler helium leaving the intermediate heat exchanger (stream 3 in **Figure 1**) is then returned through a circulator to the reactor inlet pressure and mixed with the primary coolant returning to the reactor.

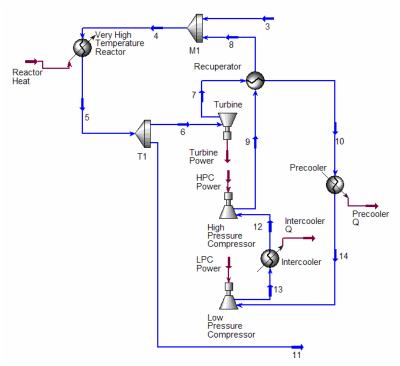


Figure 1. UniSim process flow diagram for helium recuperated direct Brayton cycle.

The reactor thermal power assumed for the high-temperature helium-cooled reactor was 600 MWt. The UniSim-calculated power cycle thermal efficiency for the system represented in **Figure 1** is 53.23 %.

3. SELECTION OF THE REFERENCE HTE PROCESS

Parametric studies evaluating the coupling of various reactor concepts with the HTE hydrogen production plant are described in References [2 and 4]. These studies included operating the HTE plant at pressures of 3.5 MPa and 7.0 MPa and with and without the use of sweep gas to remove the excess oxygen from the anode side of the electrolyzer. An integral part of all of these parametric studies was the optimization of hydrogen production rates and efficiencies using realistic operating parameters for the various components within the system.

Based on the results of these parametric studies, a gas-sweep system was selected for the reference design. While slightly higher overall hydrogen production efficiencies (1.0-1.5%) can be achieved when no gas sweep system is used, concerns with the handling of the high temperature oxygen product gas led to the decision to use a gas-sweep system for oxygen removal from the electrolyzer anode [2]. Two types of gas-sweep systems, an air-sweep and steam-sweep system were evaluated. The steam-sweep system was initially considered because of the relative ease of separating the steam and oxygen by condensation so that the oxygen product gas might be used for other commercial applications. However, the steam-sweep system

unduly complicated the design of the HTE plant and individual components and, therefore, the HTE plant with an air-sweep system was selected as the reference design.

The operating pressure of the HTE plant was also evaluated because higher operating pressures result in smaller components and/or lower system pressure drops for a given mass flow rate. However, higher system pressures also require heavier and more expensive components, and can have a negative impact on system performance and reliability. Based on these considerations, and the results of analyses performed at system operating pressures of 3.5 MPa and 7.0 MPa which indicated slightly lower overall hydrogen production efficiencies at the higher HTE operating pressure [3], an HTE operating pressure of 5.0 MPa was selected for the reference design. The decision to operate at 5.0 MPa was also influenced by the need to deliver the hydrogen gas at elevated pressure for either storage or pipeline transport. Therefore, from the standpoint of overall process efficiency, it is logical to compress the liquid water feedstock at the process inlet since liquid-phase compression work is very small compared to compression of the gaseous product. Any comparison made to the HTE reference process described here should also refer to delivery of the product hydrogen at 5.0 MPa.

A description of the reference reactor power cycle and coupled HTE hydrogen production plant based on the above considerations is provided in the following section.

4. COUPLING OF THE HTE PLANT AND REACTOR POWER CYCLE

The overall process flow diagram for the very high-temperature helium-cooled reactor coupled to the direct helium Brayton power cycle and the HTE plant with air sweep is presented in **Figure 2**. The liquid water feedstock enters at the left in the diagram. The water is then compressed to the HTE process pressure of 5.0 MPa in the liquid phase using a pump.

Downstream of the pump, condensate from the water knockout tank is recycled back into the inlet stream at M3. The water stream is then vaporized and pre-heated in the electrolysis recuperator, which recovers heat from the post-electrolyzer process and sweep-gas outlet streams. Downstream of the recuperator, at M2, the steam is mixed with recycled hydrogen product gas. A fraction of the product gas is recycled in this way in order to assure that reducing conditions are maintained on the steam/hydrogen electrode. Downstream of the mixer, the process gas mixture enters the intermediate heat exchanger (IHX), where final heating to the electrolysis operating temperature occurs, using high-temperature process heat from the nuclear reactor. The process stream then enters the electrolyzer, where oxygen is electrolytically removed from the steam, producing hydrogen and oxygen. An additional process heater is used to directly add heat during the electrolysis process to maintain isothermal electrolyzer operating conditions. The custom electrolyzer module developed at INL for direct incorporation into the UniSim system analysis code has been described in detail previously [3].

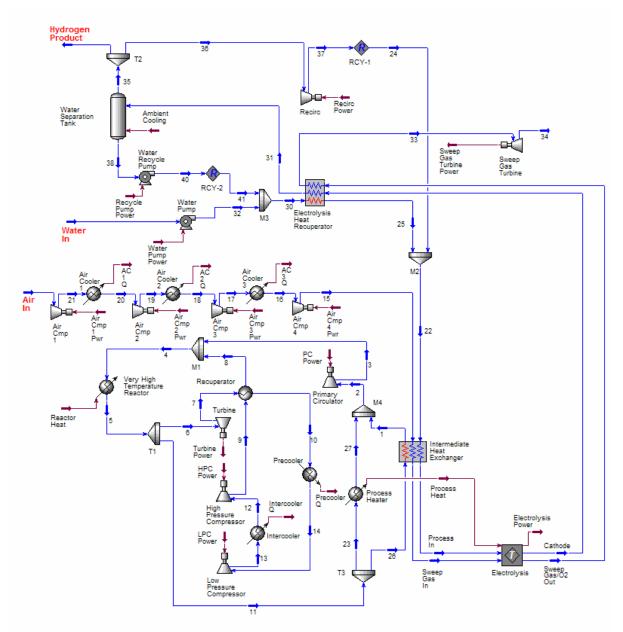


Figure 2. Process flow diagram for helium-cooled reactor/direct Brayton/HTE system with air sweep.

Downstream of the electrolyzer, the hydrogen – rich product stream flows through the electrolysis recuperator where the product stream is cooled and the inlet process stream is preheated. The product stream is cooled further at the water knockout tank, where the majority of any residual steam is condensed and separated, and yielding dry hydrogen product. The cooled product stream is split at T2 and a fraction of the product gas is recycled into the inlet process stream, as discussed previously. A recirculating blower is required to repressurize the recycle stream to the upstream pressure at M2.

The process flow diagram shows air in use as a sweep gas, to remove the excess oxygen that is evolved on the anode side of the electrolyzer. In the air sweep system, inlet air is compressed to

the system operating pressure of 5.0 MPa in a four-stage compressor with intercooling. The final compression stage is not followed by a cooler, so the air enters the IHX at about 171°C. The sweep gas is heated to the electrolyzer operating temperature of 800°C via the IHX which supplies high-temperature nuclear process heat directly to the system. The sweep gas then enters the electrolyzer, where it is combined with product oxygen. Finally, it passes through the electrolysis recuperator to help preheat the incoming process gas. Some of the sweep gas compression work is recovered using a sweep-gas turbine located at the sweep-gas exit.

5. ELECTROLYZER MODEL

The electrolyzer model process flow diagram is shown in **Figure 3**. The process flow consisting of steam and hydrogen passes through a conversion reactor where the steam is split into hydrogen and oxygen. The conversion reactor uses a stoichiometric equation for the splitting of water. Based upon the utilization, a specified percentage of the steam is converted. UniSim calculates the heat of reaction for this conversion, which is shown as the "Electrolysis Heating" energy stream in **Figure 3**. The Liquid Product stream has no flow and is really a null stream. The hydrogen, oxygen, and steam enter a component splitter labeled Electrodes. The oxygen is split from the other components and exits at anode stream. The sweep gas mixes with the anode stream and exits as the Sweep/Gas O2 Out stream. An embedded spreadsheet is used to calculate the Nernst potential, operating voltage, current and electrolysis power. In this reference case, since the boundary conditions are isothermal, the heat into the electrolysis process is also calculated.

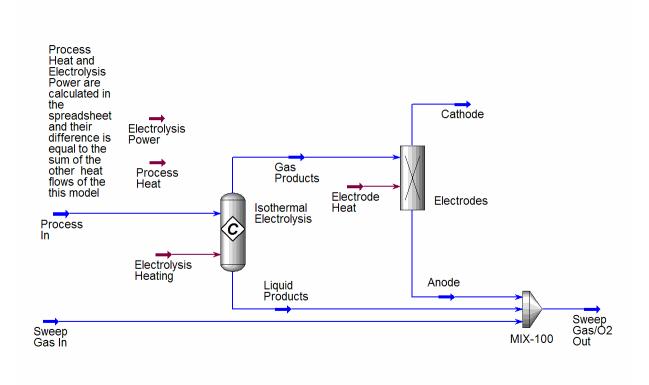


Figure 3. Process flow diagram of electrolyzer model.

Table 1 provides the flow conditions of the streams found in **Figure 3**. The composition of each stream is tabulated in Table 2. Table 3 and Table 4 display the water electrolysis reaction information.

Table 1. Electrolysis fluid stream conditions and flow rates.

Name	Vapor Fraction	Temperature (C)	Pressure (MPa)	Molar Flow (gmole/s)	Mass Flow (kg/s)
Process In	1	800	5	1521	24.97
Sweep Gas In Gas	1	800	5	1049	30.27
Products Liquid	1	800	5	2130	24.97
Products Sweep	0	800	5	0	0
Gas/O2 Out	1	800	5	1657	49.74

Table 2. Mole fraction composition data for electrolysis unit.

Tuble 2. Whole fraction composition data for electrolysis unit.							
Name	H2O	Hydrogen	Oxygen	Nitrogen	CO2	Helium	
Process In	0.9	0.1	0	0	0	0	
Sweep Gas							
In	0	0	0.21	0.79	0	0	
Gas							
Products	0.0714	0.6429	0.2857	0	0	0	
Liquid							
Products	0.0714	0.6429	0.2857	0	0	0	
Sweep							
Gas/O2 Out	0	0	0.5	0.5	0	0	
Cathode	0.1	0.9	0	0	0	0	
Anode	0	0	1	0	0	0	

Table 3. Isothermal electrolysis reaction (88.89% water conversion).

Component	Mole Weight	Stoichiometric Coeff.
Hydrogen	2.016	2
Oxygen	32	1
H2O	18.02	-2

Table 4. Isothermal flow and reaction balance (88.89% water conversion).

Components	Total Inflow (gmole/s)	Total Reaction (gmole/s)	Total Outflow (gmole/s)
H2O	1369	-1217	152.1
Hydrogen	152.1	1217	1369
Oxygen	0	608.4	608.4
Nitrogen	0	0	0
CO2	0	0	0
Helium	0	0	0

6. OPTIMIZATION OF REFERENCE DESIGN

Optimization of the reference design was performed as part of the parametric studies in Reference [2]. The methodology and constraints used in running the UniSim simulations in order to maximize hydrogen production efficiencies for the very high-temperature helium-cooled reactor coupled to the direct helium Brayton power cycle and the HTE plant were as follows:

- 1. Specify desired current density, inlet and outlet compositions of steam and hydrogen, cell area and total number of cells. We have specified 90% steam, 10% hydrogen at the inlet and 10% steam, 90% hydrogen at the outlet. This corresponds to a steam utilization of 88.9%.
- 2. Determine the required mass flow rate of process steam based on the specified current density (and corresponding hydrogen production rate) and inlet and outlet compositions.
- 3. Adjust the flow split at T2 to achieve the desired inlet composition (10% hydrogen, 90% steam)
- 4. For the air sweep system, the mass flow of the air is automatically adjusted to produce an outlet stream that is 50% oxygen (the remainder is nitrogen).
- 5. Adjust the outlet pressure of the low-pressure compressor to achieve maximum power-cycle efficiency.
- 6. Adjust the power cycle/HTE process heat split at T1 to maximize hydrogen production efficiency until the minimum approach temperature of the electrolysis heat recuperator is just below 50°C.
- 7. Assume the power cycle turbine adiabatic efficiency is 93%. Power cycle compressor efficiencies are 88%. All other compressor, turbine and pump efficiencies are 75%.

Using the above approach, the per-cell active area for electrolysis was assumed to be 225 cm². This cell size is well within the limits of current technology for planar cells. The total number of cells used in the reference design was determined by specifying a current density of 0.25 amperes/cm² for an area-specific resistance, ASR, value of 0.4 and assuming isothermal conditions for the electrolysis process. The number of cells was adjusted until the full power cycle output at this operating point is dedicated to electrolysis. This procedure resulted in 4.176 x 10^6 cells required.

The ASR value of 0.4 used in the electrolyzer model is based on the current best achievable ASR for solid oxide fuel cells [5].

To allow for comparisons between the performances of the HTE process to alternate hydrogen production techniques, we have adopted a general efficiency definition that can be applied to any thermal water-splitting process, including HTE, low-temperature electrolysis (LTE), and thermochemical processes. Since the primary energy input to the thermochemical processes is in the form of heat, the appropriate general efficiency definition to be applied to all of the techniques is the overall thermal-to-hydrogen efficiency, η_H . This efficiency is defined as the heating value of the produced hydrogen divided by the total thermal input required to produce it. In this report, the lower heating value, LHV, of the produced hydrogen has been used:

$$\eta_H = \frac{LHV}{\sum_i Q_i} \tag{1}$$

The denominator in this efficiency definition quantifies all of the net thermal energy that is consumed in the process. For a thermochemical process, this summation includes the direct nuclear process heat as well as the thermal equivalent of any electrically driven components such as pumps, compressors, etc. The thermal equivalent of any electrical power consumed in the process is the power divided by the thermal efficiency of the power cycle. For the reference helium-cooled direct Brayton cycle, the power-cycle thermal efficiency is 53.2%. For the electrolysis process, the summation in the denominator of Eqn. (1) includes the thermal equivalent of the primary electrical energy input to the electrolyzer and the secondary contributions from smaller components such as pumps and compressors. In additional, any direct thermal inputs are also included. Direct thermal inputs include any net (not recuperated) heat required to heat the process streams up to the electrolyzer operating temperature and any direct heating of the electrolyzer itself required for isothermal operation. Finally, if a reactor outlet temperature is insufficient to raise the feed temperature to the desired electrolyzer operating temperature (in this case 800° C), then the thermal equivalent of any auxiliary heaters must be included. If these heaters use electrical resistance heat, the heat input is penalized by the power cycle thermal efficiency. If the heaters are combustion-based, only the direct heat amount is included.

7. REFERENCE DESIGN CONDITIONS

Fluid conditions, flow rates, stream composition and component operating parameters for the optimized reference case are summarized in Tables 5-11 at each of the locations shown in Figure 2. The temperature, pressure, molar and mass flow rates, and the vapor fraction for each stream are displayed in Table 5. The composition of each stream is shown in Table 6. Table 7 provides the heat rates and the electrolysis power shown in Figure 2. The thermal duty, overall heat transfer coefficient, UA, log-mean temperature difference, LMTD, and the minimum approach temperature for each heat exchanger is found in Table 8. Turbine, compressor and pump parameters are given in Tables 9-11. Figures 4, 5, and 6 show temperature versus heat flow profiles of the recuperator, IHX, and electrolysis heat recuperator heat exchangers. Figure 4 shows that the recuperator has a very tight profile. The minimum temperature difference is 17 °C. The temperature profile of the IHX is shown in **Figure 5**. The cold side profile is a composite of the air sweep and the process streams. This heat exchanger has a temperature difference of 100 °C due to the temperature difference between the outlet of the reactor, 900 °C and the electrolysis process temperature, 800 °C. The electrolysis heat recuperator profile is found in **Figure 6**. This profile has a minimum approach temperature of 50 °C. The cold stream is the water entering the process. The hot side is a composite of the sweep gas and the process gas after electrolysis. One can see that the water starts at a sub-cooled state and ends at a superheated state. The temperature profiles reveal that there are no temperature crossovers; therefore the heat exchangers should operate effectively.

Table 5. Stream fluid conditions and flow rates for reference plant design.

1 able 5. Stream		naitions and			
Name	Vapor Fraction	Temperature (C)	Pressure (MPa)	Molar Flow (gmole/s)	Mass Flow (kg/s)
Process In	1	800	5	1521	24.97
Sweep Gas In	1	800	5	1049	30.27
Sweep Gas/O2 Out	1	800	5	1657	49.74
Cathode	1	800	5	1521	5.5
2	1	515.723	6.949	1.07E+04	42.73
3	1	523.013	7.07	1.07E+04	42.73
4	1	540	7.07	8.01E+04	320.5
5	1	900	7.019	8.01E+04	320.5
6	1	900	7.019	6.94E+04	277.8
_ 7	1	560.506	2.763	6.94E+04	277.8
8	1	542.613	7.07	6.94E+04	277.8
9	1	100.098	7.18	6.94E+04	277.8
10	1	117.509	2.713	6.94E+04	277.8
11	1	900	7.019	1.07E+04	42.73
12	1	26	4.387	6.94E+04	277.8
13	1	100.029	4.407	6.94E+04	277.8
14	1	26	2.693	6.94E+04	277.8
15	1	170.566	5.035	1049	30.27
16	1	46.85	2.034	1049	30.27
17	1	176.85	2.054	1049	30.27
18	1	46.85	0.7962	1049	30.27
19	1	176.85	0.8047	1049	30.27
20	1	46.85	0.3117	1049	30.27
21	1	176.85	0.3147	1049	30.27
Air In	1	26.85	0.1013	1049	30.27
22	1	317.954	5.035	1521	24.97
25	1	344.319	5.035	1369	24.66
30	0	17.0668	5.07	1369	24.66
32	0	15.9666	5.07	1219	21.96
Water In	0	15.5556	0.1013	1219	21.96
31	0.9102	80.3227	4.965	1521	5.5
33	1	148.147	4.965	1657	49.74
34	1	-66.032	0.1013	1657	49.74
36	1	26	4.965	152.2	0.3089
37	1	27.6446	5.035	152.2	0.3089
38	0	26	4.965	151	2.72
Hydrogen Product	1	26	4.965	1218	2.472
40	0	26.0091	5.07	151	2.72
41	0	26.0091	5.07	150	2.703
35	1	26	4.965	1370	2.781
24	1	27.6446	5.035	152.2	0.3089
_ 1 _	1	515.723	6.949	6387	25.57
23	1	900	7.019	4287	17.16
26	1	900	7.019	6387	25.57
27	1	515.723	6.949	4287	17.16

Table 6. Mole fraction composition data for reference plant design

Table 6. Mole fract		sition data fo	or reference			
Name	H2O	Hydrogen	Oxygen	Nitrogen	CO2	Helium
Process In	0.9	0.1	0	0	0	0
Sweep Gas In	0	0	0.21	0.79	0	0
Sweep Gas/O2 Out	0	0	0.5	0.5	0	0
Cathode	0.1	0.9	0	0	0	0
2	0	0	0	0	0	1
3	0	0	0	0	0	1
4	0	0	0	0	0	1
5	0	0	0	0	0	1
6	0	0	0	0	0	1
7	0	0	0	0	0	1
8	0	0	0	0	0	1
9	0	0	0	0	0	1
10	0	0	0	0	0	1
11	0	0	0	0	0	1
12	0	0	0	0	0	1
13	0	0	0	0	0	1
14	0	0	0	0	0	1
15	0	0	0.21	0.79	0	0
16	0	0	0.21	0.79	0	0
17	0	0	0.21	0.79	0	0
18	0	0	0.21	0.79	0	0
19	0	0	0.21	0.79	0	0
20	0	0	0.21	0.79	0	0
21	0	0	0.21	0.79	0	0
Air In	0	0	0.21	0.79	0	0
22	0.9	0.1	0	0	0	0
25	1	0	0	0	0	0
30	1	0	0	0	0	0
32	1	0	0	0	0	0
Water In	1	0	0	0	0	0
31	0.1	0.9	0	0	0	0
33	0	0	0.5	0.5	0	0
34	0	0	0.5	0.5	0	0
36	0.0008	0.9992	0	0	0	0
37	0.0008	0.9992	0	0	0	0
38	0.9999	0.0001	0	0	0	0
Hydrogen Product	0.0008	0.9992	0	0	0	0
40	0.9999	0.0001	0	0	0	0
41	0.9999	0.0001	0	0	0	0
35	0.0008	0.9992	0	0	0	0
24	0.0008	0.9992	0	0	0	0
1	0	0	0	0	0	1
23	0	0	0	0	0	1
26	0	0	0	0	0	1
27	0	0	0	0	0	1

Table 7. Component heat rates and electrolysis power for reference design.

Name	Heat Flow (kW)
Process Heat	3.43E+04
Reactor Heat	6.00E+05
Intercooler Q	1.07E+05
Precooler Q	1.32E+05
AC 3 Q	4134
AC 2 Q	4083
AC 1 Q	4062
Ambient Cooling	-3370
Electrolysis Power	-2.69E+05

Table 8. Heat exchanger design parameters for reference plant design.

Name	Duty (kW)	UA (W/C)	LMTD (C)	Minimum Approach (C)
Recuperator	-6.40E+05	3.62E+07	17.7	17.41
Intermediate Heat Exchanger	5.11E+04	3.14E+05	162.6	100
Electrolysis Heat Recuperator	7.44E+04	6.39E+05	116.4	50

Table 9. Turbine design parameters for reference plant design.

Name	Adiabatic Efficiency	Polytropic Efficiency	Power (kW)
Turbine	93	92	4.91E+05
Sweep Gas Turbine	75	62	1.01E+04

Table 10. Compressor design parameters for reference plant design.

Name	Adiabatic Efficiency	Power (kW)
Primary Circulator	75	1622
High Pressure		
Compressor	88	1.07E+05
Low Pressure		
Compressor	88	1.07E+05
Air Cmp 4	75	3851
Air Cmp 3	75	4047
Air Cmp 2	75	4048
Air Cmp 1	75	4661
Recirc	75	7.21

Table 11. Pump design parameters for reference plant design.

Name	Adiabatic Efficiency (%)	Power (kW)	Pressure Head (m)
Water Pump	75	143.4	499.5
Water Recycle Pump	75	0.3778	10.62

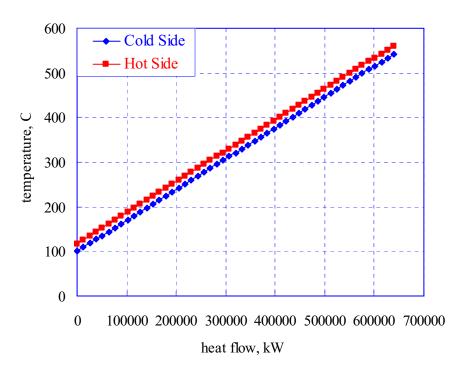


Figure 4. Temperature profile plot of Brayton cycle recuperator.

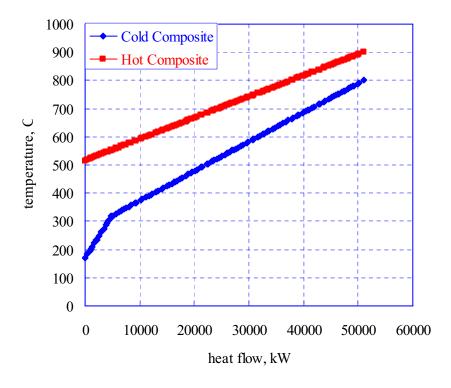


Figure 5. Temperature profile of Intermediate Heat Exchanger.

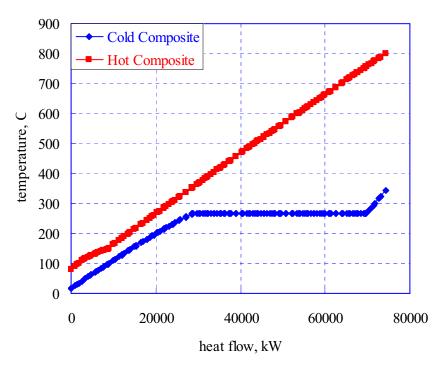


Figure 6. Temperature profile of Electrolysis Heat Recuperator.

A parametric study was also performed using the reference model. In one study, the current density was adjusted while keeping the steam utilization constant at 88.9%. This study also kept the electrolysis process isothermal thus requiring direct heat from the reactor if the current density is below thermal neutral or heat rejection from the electrolysis process if the current density is above thermal neutral. **Figure 7** is a plot of the resulting overall hydrogen production efficiency as a function of the hydrogen production rate (top axis) or the current density (bottom axis). As can be seen in the figure, the hydrogen production rate has a direct relationship to the current density given a constant cell area and number of cells. The overall hydrogen production efficiency increases as the current density decreases which also corresponds to a decrease in the hydrogen production rate.

A second parametric study was performed by setting the process and air sweep flow rates constant, which results in variable steam utilization. In this study, adiabatic boundary conditions were set with respect to the electrolysis process. The current density was again adjusted. **Figure 8** shows the overall hydrogen production efficiency as a function of the steam utilization. As the current density decreases, the steam utilization decreases because the process stream flow rate remains constant. Lower current density means less steam is converted to hydrogen and oxygen for a given flow rate of water. **Figure 8** shows that at lower steam utilization, the overall hydrogen production efficiency decreases rapidly, especially below about 40% utilization.

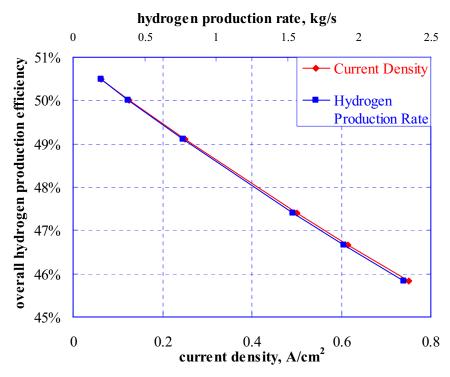


Figure 7. Overall hydrogen product efficiency as a function of current density for an ASR of 0.4, isothermal boundary conditions, and constant steam utilization.

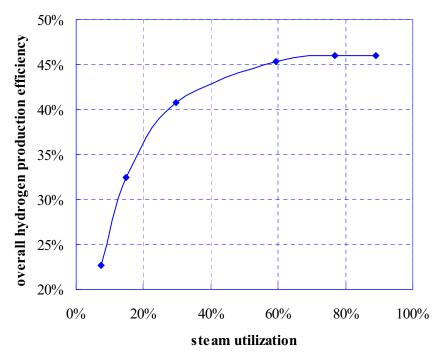


Figure 8. Overall hydrogen production efficiency as a function of steam utilization for an ASR of 0.4, adiabatic boundary conditions, and constant process and air sweep flows.

8. CONCLUSIONS

This report presents results from the optimization of a reference commercial-scale high-temperature electrolysis (HTE) plant for hydrogen production. The reference HTE plant is driven by a 600 MWt high-temperature helium-cooled reactor coupled to a direct Brayton power cycle with a reactor outlet temperature of 900° C. The reference plant optimization is based on previous parametric studies performed using the UniSim process analysis software [3, 4].

The reference plant simulation was performed for a cell area-specific resistance value of 0.4 Ohm·cm². The ASR value of 0.4 represents a stack-average ASR value that should be achievable in the short term with existing technology. Isothermal operation of the electrolyzer was assumed. An air sweep system is also included in the reference design to remove oxygen from the anode side of the electrolyzer because of concerns with handling of the high-temperature oxygen product gas. Predicted overall thermal-to-hydrogen efficiency values for the reference design with an air-sweep system resulted in hydrogen production efficiencies that were only 1.0 – 1.5 percentage points lower than the equivalent design with no sweep-gas system [2]. The operating pressure of 5.0 MPa for the HTE process loop was selected to be consistent with the need to deliver the hydrogen product gas at elevated pressures for storage or pipeline transport. This pressure also represents a trade off between the need for larger components at lower pressures and the need for more massive components for pressure containment at higher pressures.

The simulation for the reference HTE plant coupled to the helium recuperated Brayton cycle indicated a power-cycle thermal efficiency of 53.2%. Earlier parametric studies predicted overall hydrogen production efficiencies in the 45 - 50% range depending on the assumed current density [2]. These same studies also indicated that for adiabatic operation of the electrolyzer, a nonlinear decrease in overall hydrogen production efficiency occurred with increasing current density, as a result of the temperature-dependent *ASR* used in the simulation.

The information presented in this report is intended to establish an optimized design for the reference nuclear-driven HTE hydrogen production plant so that parameters can be compared with other hydrogen production methods and power cycles to evaluate relative performance characteristics and plant economics.

9. REFERENCES

- 1. Herranz, L. E., Linares, J. I., and Moratilla, B. Y., "Assessment of regenerative reheating in direct Brayton power cycles for high-temperature gas-cooled reactors," *Nuclear Technology*, v 159, n 1, July, 2007, pp. 15-24.
- 2. McKellar, M. G., O'Brien, J. E., Herring, J. S., "Commercial Scale Performance Predictions for High-Temperature Electrolysis Plants Coupled to Three Advanced Reactor Types", INL Internal Report, September 14, 2007.
- 3. O'Brien, J. E., Stoots, C. M., and Hawkes, G. L., "Comparison of a One-Dimensional Model of a High-Temperature Solid-Oxide Electrolysis Stack with CFD and Experimental Results," Proceedings, 2005 ASME International Mechanical Engineering Congress and Exposition, Nov. 5 11, Orlando.
- 4. Harvego, E. A., McKellar, M. G., O'Brien, J. E., and Herring, J. S., "Summary of Reactor-Coupled HTE Modeling Sensitivity Studies," DOE Milestone Report, October 26, 2006.
- 5. Surdoval, Wayne, Nuclear Hydrogen Initiative Semiannual Program Review, October 24, 2007, Red Lion Hotel, Idaho Falls, Idaho.