HYDROGEN PRODUCTION USING A SUPERCritical CO2-COOLED FAST REACTOR AND STEAM ELECTROLYSIS

by

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B.S., Chemical Engineering (2005)

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Submitted to the Department of Nuclear Science and Engineering in Partial Fulfillment of the Requirements for the Degree of Master of Science in Nuclear Science and Engineering

at the

Massachusetts Institute of Technology

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Abstract

Rising natural gas prices and growing concern over CO₂ emissions have intensified interest in alternative methods for producing hydrogen. Nuclear energy can be used to produce hydrogen through thermochemical and/or electrochemical processes.

This thesis investigates the feasibility of high temperature steam electrolysis (HTSE) coupled with an advanced gas-cooled fast reactor (GFR) utilizing supercritical carbon dioxide (S-CO₂) as the coolant. The reasons for selecting this particular reactor include fast reactor uranium resource utilization benefits, lower reactor outlet temperatures than helium-cooled reactors which ameliorate materials problems, and reduced power conversion system costs.

High temperature steam electrolysis can be performed at conditions of 850°C and atmospheric pressure. However, compression of the hydrogen for pumping through pipes is unnecessary if electrolysis takes place at around 6 MPa. The reactor coolant at 650°C is used to heat the steam up to temperatures ranging between 250°C and 350°C, and the remaining heat is provided by thermal recuperation from product hydrogen and oxygen.

Several different methods for integrating the hydrogen production HTSE plant with the GFR were investigated. The two most promising methods are discussed in more detail: extracting coolant from the power conversion system (PCS) turbine exhaust to boil water, and extracting coolant directly from the reactor using separate water boiler (WB) loops. Both methods have comparable thermal to electricity efficiencies (~43%) at 650°C. This relates to an overall hydrogen production efficiency of about 47%. The approach which utilizes separate WB loops has the added advantage of being able to provide emergency cooling to the reactor, and also the benefit of not interfering with the operation of the PCS. This makes the separate WB loop integration method a more desirable scheme for hydrogen production using HTSE.

The HTSE electrolysis unit adopted for the present analysis was designed by Ceramatec in coordination with INL. In this unit the steam flows into an electrolytic cell. It is separated by electron flow from a nickel-zirconium cathode to a strontium-doped lanthanum manganite anode. The optimal conditions for stack operation have been found by INL using various modeling and experimental techniques. These conditions include a 10% by volume flow of hydrogen in the feed, a stack operating temperature of 800°C, and an operating voltage of 1.2 V.

The GFR integrated with the HTSE plant via separate water boiler loops was modeled in this work using the chemical engineering code ASPEN. The results of this
model were benchmarked against the Idaho National Lab (INL) process, modeled using HYSIS. Both models predict a hydrogen production rate of \( \sim 10.2 \text{ kg/sec (} \pm 0.2 \text{ kg/sec)} \) for a 600 MW\text{th} reactor with an overall efficiency ranging between 47\%-50\%. The highly recuperated HTSE plant developed for the GFR can in principle be used in conjunction with a variety of other nuclear reactors, without requiring high reactor coolant outlet temperatures.

**Thesis Supervisor:** Michael J. Driscoll  
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I would like to acknowledge the Idaho National Laboratory, whose research, modeling, and development of the experimental HTSE unit in conjunction with Ceramatec Inc. provided critical data and benchmarking for this thesis.

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Hydrogen Production Using a Supercritical CO₂-Cooled Fast Reactor and Steam Electrolysis

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Chapter 1 Introduction

Hydrogen plays an important role in many potential sustainable energy scenarios. Worldwide energy demand and consumption are increasing at an exponential rate, while the world fossil fuel reserves that currently play the primary role of energy provision are depleting at an ever increasing rate. This indicates that to support the rising demand, better utilization of the chemical energy stored within hydrocarbon fossil fuels must be employed and/or substitutes developed. In addition, increasing carbon dioxide emissions from the combustion of fossil fuels is driving an effort to find alternative energy resources.

Hydrogen has been identified as one of the potential solutions to the growing energy problem. This is due to hydrogen’s potential to be used as a clean, environmentally friendly and relatively safe-to-handle energy carrier for several different applications [1.1][1.2]. As a consequence, using nuclear energy to produce hydrogen is a technology that has gained international attention. This work focuses on producing hydrogen through nuclear means. As will be seen, this requires either very high temperatures for thermochemical processes or highly efficient generation of electricity for electrolytic processes: both approaches can be realized by the use of gas cooled reactors. Accordingly, to meet the objectives of the NERI project which supports this work, an integrated system for producing nuclear hydrogen using a Generation IV gas-cooled fast reactor, cooled by supercritical carbon dioxide coupled with an innovative solid oxide cell high temperature steam electrolysis unit, is devised and evaluated in this thesis.
1.1 Objectives and Scope

Previous papers have identified methods for producing hydrogen, identified hydrogen demand, and performed preliminary calculations identifying the feasibility of overall hydrogen production, as well as outlining the scope of the hydrogen economy [3.1]. The objective of this thesis is to maximize the process efficiency for the production of nuclear hydrogen. Several methods for producing hydrogen have been identified, but the focus of this thesis will be on using High Temperature Steam Electrolysis (HTSE). Several possible reactor types have been proposed for use with a hydrogen production unit, and we have chosen to focus our work on utilizing a moderate temperature (~650°C) gas cooled reactor in conjunction with the HTSE unit. The properties of several gas cooled reactors that are appropriate for use in coordination with a high temperature electrolysis unit are discussed, and based upon the considerations given, a supercritical carbon dioxide cooled gas-cooled fast reactor (S-CO₂-GFR) is selected as the reference concept.

Previous work performed at MIT has identified a preliminary layout for an S-CO₂-GFR/HTSE integrated plant [3.2]. The work described in this thesis has accomplished two further primary objectives: the identification of an optimal system of integration between the S-CO₂-GFR and the HTSE plant, and the maximization of the thermal recuperation for the overall nuclear hydrogen system. The first objective was realized by careful study of the thermodynamic, safety, and materials development properties of several different plant design layouts. The design layouts studied include,
but are not restricted to, the two primary designs discussed in this thesis: providing feedwater to the HTSE unit, boiled by extracting S-CO$_2$ from the turbine exhaust of the power conversion system (PCS) of the primary loops; versus providing feedwater to the HTSE unit, boiled by extracting S-CO$_2$ directly from the reactor itself in separate water boiler loops. The maximization of thermal recuperation was performed by studying the possible design locations where heat was available for recovery, and by calculating the heat recuperation possible for each of these heat sources.

1.2 Hydrogen Demand

Over the past several decades a number of studies have identified the potential for hydrogen, and the value of a hydrogen economy [1.3][1.4]. There are three basic areas with potential for hydrogen demand based upon ability to produce cheap hydrogen: 1) transportation needs, 2) stationary power needs, and 3) industrial uses [1.5]. Each of these areas can, for example, utilize fuel cell technology to match energy consumption demands.

Hydrogen use in the transportation sector is a difficult area to address; the transportation sector is a complex system involving public and private involvement that is already heavily dependent upon liquid fuels. To transfer the entire network of public transportation including ground, air and water, to a system based upon hydrogen rather than liquid fuels would be a costly task due in particular to the geographically diffuse nature of the system. If that direction is pursued, however, fuel cells provide an attractive alternative to liquid fossil fuel consumption for the transportation sector. Fuel cells
convert hydrogen and oxygen into water, releasing energy in a reaction similar to the reverse of the HTSE reaction discussed in chapter 4. The success of fuel cells in the transportation sector will depend on the availability and cost of hydrogen in addition to the success in creating compact fuel cells with optimal power generation capacity.

Hydrogen demand in the stationary power sector is a more reasonable application [1.6]. The stationary power option doesn’t require a restructuring of the entire power network, as fuel cells in the transportation sector would. Two primary methods could be employed to provide power using hydrogen. One is to directly combust hydrogen gas. Current gas turbines with conventional gas combustion systems can operate on H₂ with very little modification of the system [1.5]. This option is favorable, because unlike fossil fuel combustion, hydrogen combustion releases only water as its byproduct, with no carbon dioxide emissions. Because no major modifications to existing gas turbines are required, direct fired hydrogen could provide an early market for hydrogen. The greatest disadvantage to direct fired hydrogen combustion plants is the large volume of hydrogen required to fuel the plant. The volumetric heating value for hydrogen is around 11 kJ/N-m³, as compared to 36 kJ/N-m³ for methane. This means nearly 3.32 times the volume of hydrogen would be needed for a comparable energy output [1.5].

A much more promising method for stationary energy production is the use of stationary fuel cell systems. Similar to direct fired power production plants, fuel cell systems would generate safe, clean, and efficient power with no carbon emissions. The largest barrier to widespread fuel cell use in the stationary power production sector is the cost. Capital costs are nearly four times more than for ICE generators. There are several different types of fuel cells, differing in both construction and material composition. A
listing of some of the current models for fuel cell stationary power production is given in Table 1.1. It is a common belief that fuel cell performance and

<table>
<thead>
<tr>
<th>Cost and Performance Characteristics</th>
<th>System 1</th>
<th>System 2</th>
<th>System 3</th>
<th>System 4</th>
<th>System 5</th>
<th>System 6</th>
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<tbody>
<tr>
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<td>PEMFC</td>
<td>MCFC</td>
<td>MCFC</td>
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</tr>
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<tr>
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<td>35</td>
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<td>69</td>
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<td>70</td>
<td>70</td>
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<td>1360</td>
<td>1170</td>
<td>950</td>
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<td>59.3</td>
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<td>65.5</td>
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<td>Commercial status, 2003</td>
<td>Commercially available</td>
<td>Demonstration</td>
<td>Demonstration</td>
<td>Commercially introduced</td>
<td>Demonstration</td>
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</table>

NOTE: PAFC = phosphoric acid fuel cell; PEMFC = proton exchange membrane fuel cell; MCFC = molten carbonate fuel cell; SOFC = solid oxide fuel cell; CHP = combined heat and power; HHV = higher heating value.

design will dramatically improve within the next few years due to the heavy federal R&D funding focused on improving the technology [1.5]. A summary of the projected properties of stationary power fuel cells in the year 2020 is given in Table 1.2. If the
predicted trend continues, the hydrogen fuel cell could be a competitive power source in the near future, ensuring a continued demand for cheap hydrogen.

Table 1.2: Stationary Fuel Cell Systems—Projected Typical Performance Parameters in 2020 [1.3]

<table>
<thead>
<tr>
<th>Cost and Performance Characteristics</th>
<th>System 1</th>
<th>System 2</th>
<th>System 3</th>
<th>System 4</th>
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<td>PEMFC</td>
<td>PEMFC</td>
<td>MCFC</td>
<td>MCFC</td>
<td>SOFC</td>
</tr>
<tr>
<td>System size (kW)</td>
<td>--</td>
<td>10</td>
<td>200</td>
<td>250</td>
<td>2000</td>
<td>100</td>
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<tr>
<td>Total installed cost ($/kW)</td>
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<td>51</td>
</tr>
<tr>
<td>Total CHP efficiency (%)</td>
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<td>72</td>
<td>75</td>
<td>75</td>
<td>72</td>
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<tr>
<td>Effective electrical efficiency (%)</td>
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<td>65</td>
<td>71</td>
<td>73</td>
<td>69</td>
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</table>

NOTE: PAFC = phosphoric acid fuel cell; PEMFC = proton exchange membrane fuel cell; MCFC = molten carbonate fuel cell; SOFC = solid oxide fuel cell; CHP = combined heat and power; HHV = higher heating value.

Commercial chemical process plant use of hydrogen is currently the largest demand for hydrogen. Over 300 trillion standard cubic feet (scf) of hydrogen are used each year. Currently, these uses include ammonia production, methanol production, hydrocarbon refining, reagents for other chemical production processes, and other uses [1.6]. The proportions of these uses are shown in Fig. 1.1. The future demand for hydrogen in industry would include the uses already listed, but on a larger scale as each of these industries expand. In addition, direct combustion of hydrogen could be
incorporated into the industrial processes to fuel furnaces and other heat sources. This would result in an improved efficiency (99% up from about 80% for current processes), decreasing the operational costs of industrial processes.

Figure 1.1: Global uses for hydrogen in industry currently

An additional and promising demand for hydrogen could emerge in the near future as a better energy option for the transportation sector. This alternative involves the combination of hydrogen and carbon monoxide to produce synthetic liquid fuels, such as methanol [1.7]. Several paths and reactions could be used to produce these synthetic fuels, which could be used in exactly the same conditions and circumstances as current liquid fuels. Because this option doesn’t depend on changing the transportation fuel source network, it is more plausible than a direct hydrogen economy. Fig. 1.2 shows
some of the pathways to synthetic fuels using hydrogen gas and biomass as reagents that are being investigated by the INL [4.9]. Any of these processes could be used to produce synthetic fuels cheaply and efficiently, further increasing the demand for hydrogen in producing energy for the transportation sector. Finally, hydrogen can be used to upgrade heavy oils, tar sands, shale oil, and the like. While this could well be a large near term application, we will not examine these options further in this thesis, because it would result in increased CO₂ emissions.

Figure 1.2: Pathways from Biomass to Liquid fuels using hydrogen gas [4.9]
1.3 Hydrogen Production

Currently, hydrogen is produced primarily through methane reformation. Other methods include hydrogen production from coal, oil, and electrolysis of water [1.6]. The fractional production of hydrogen from each method is summarized in Fig. 1.3.

Approximately 48% of the hydrogen produced in the world is through the process in which steam and methane are reacted over a nickel catalyst [1.8]. This process, in addition to processes involving gas and coal, provides the large majority of hydrogen produced worldwide (~96%). Increasing concerns over the carbon dioxide produced by these methods, however, have driven a major effort to develop alternative cost-effective hydrogen production methods. Many of these advanced hydrogen production methods...
involve the use of nuclear energy at some point in the hydrogen production process. The most promising of the nuclear hydrogen methods are high temperature electrolysis, high pressure electrolysis, the sulfur-iodine process, and steam methane reforming using nuclear heat. An economic comparison of each of these processes along with steam

Table 1.3: Economic comparison of several nuclear hydrogen production processes [4,9]

<table>
<thead>
<tr>
<th>Process</th>
<th>Energy Source</th>
<th>Reactor Core Outlet Temp., °C</th>
<th>Process Max. Cycle Temp., °C</th>
<th>( H_2 ) Cost w/o ( O_2 ) Credit, $/kg</th>
<th>( H_2 ) Cost with ( O_2 ) Credit, $/kg</th>
</tr>
</thead>
<tbody>
<tr>
<td>High Pressure Electrolysis</td>
<td>Gas Turbine-HTGR</td>
<td>850</td>
<td>80</td>
<td>$ 2.45</td>
<td>$ 2.29</td>
</tr>
<tr>
<td>Steam Methane Reforming*</td>
<td>Natural Gas</td>
<td>NA</td>
<td>700</td>
<td>$ 1.35</td>
<td>--</td>
</tr>
<tr>
<td>Steam Methane Reforming*</td>
<td>Process Heat-HTGR</td>
<td>850</td>
<td>700</td>
<td>$ 1.20</td>
<td>--</td>
</tr>
<tr>
<td>Sulfur-Iodine</td>
<td>Process Heat-HTGR</td>
<td>1000</td>
<td>900</td>
<td>$ 2.07</td>
<td>$ 1.91</td>
</tr>
<tr>
<td>High Temperature Electrolysis</td>
<td>HTGR</td>
<td>1000</td>
<td>850</td>
<td>$ 2.31</td>
<td>$ 2.15</td>
</tr>
</tbody>
</table>

source: EPRI 1000687, Oct 2004

* natural gas:$5.60/million BTU, sequestration: $4.09/MT \( CO_2 \)

methane reforming is shown in Table 1.3. Although currently steam methane reforming without nuclear heat is the cheapest option, rising natural gas costs and the possibility of carbon emissions taxation could make the other options much more appealing.

Of the hydrogen production processes listed in Table 1.3, only the electrolysis methods, and the sulfur-iodine method produce no carbon emissions. High pressure electrolysis is more expensive than high temperature electrolysis, and much less developed. Therefore, the two primary methods under investigation for hydrogen
production are the Sulfur-Iodine (SI) process and the High Temperature Steam Electrolytic (HTSE) process.

1.3.1 The Sulfur-Iodine Process

The SI process is depicted in Figure 1.4. This process is a three step reaction process which utilizes nuclear heat to reach the desired reaction temperatures. The first reaction requires high quality heat at 900°C which will be provided by a nuclear reactor. In this reaction, sulfuric acid decomposes into oxygen, sulfur dioxide, and steam. The

![Conceptual Schematic of the SI process for hydrogen production](image)

**Figure 1.4: Conceptual Schematic of the SI process for hydrogen production [4.9]**
product stream from this reaction is oxygen, while the steam and sulfur dioxide are fed into the heat-rejecting reaction. The second reaction of this process is a cooler reaction, taking place at only 400°C (also supplied by the nuclear reactor). In this reaction, hydrogen iodide decomposes into hydrogen and iodine. The hydrogen is recovered as the product stream, while the iodine is fed into the heat-rejecting reaction. The final reaction, the heat rejecting reaction, involves combining iodine, steam, and sulfur dioxide at 100°C to create hydrogen iodide and sulfuric acid. These two products are then heated using nuclear process heat and fed back into their respective chemical reactors.

The sulfur-iodine process is more attractive than other methods of nuclear hydrogen production primarily due to its high efficiency of around 50% [1.9]. However, there are some major drawbacks to this method. The first is the complexity of the process. Three different reactions, and thus three different plant stages, are required. The second is that some of the components involved, such as iodine and sulfur dioxide are highly toxic, and could pose significant safety hazards in an accident scenario. Finally, an integrated pilot scale demonstration of this process has yet to be conducted; no data has been obtained yet to determine if this process will be feasible as currently envisioned. For example, several recent conceptual designs indicate a very large electrical power demand by the SI plant, with 30 to 45% of the total thermal energy required to produce the electricity for powering pumps and compressors [1.10]. Also, efficiency drops rapidly as the electrolysis temperature decreases, but high temperatures pose a significant materials corrosion problem.
1.3.2 High Temperature Steam Electrolysis

The high temperature steam electrolysis (HTSE) method for producing hydrogen involves using high temperature steam as a feed. The steam is raised to electrolytic conditions using nuclear heat, and is reacted in a single stage electrolytic cell. This process if coupled with a high efficiency HTGR reaches efficiencies nearly comparable to the sulfur iodine process (~45-51%) [3.1] but takes place in a single stage without any toxic reagents or costly components or catalysts. The electrolytic cell is relatively small, cheap, and easy to construct, and has been tested in small scale experimental runs. Because of these advantages, the focus of this thesis will be the implementation of HTSE for producing hydrogen using nuclear heat. The details and schematics of this process will be discussed in greater detail in chapter 4.

1.4 Supercritical CO$_2$ Plant

In order to provide sufficiently high temperatures to the electrolysis unit together with highly efficient generation of electricity, care should be taken in selecting an appropriate reactor for integration with the hydrogen production plant. Possible gas reactors include the very high temperature reactor (VHTR), an AGR coupled to the S-CO$_2$ cycle, the gas cooled fast reactor (GFR) cooled by helium, and the GFR cooled by supercritical CO$_2$ (S-CO$_2$). The reactor selected for use in this work is the S-CO$_2$-GFR,
though either of the other two reactors (and several others) could similarly be used. The motivation for selecting the S-CO$_2$-GFR is due to its efficiency and cost-effective design. A more full discussion is given in chapter 2 of this thesis.

Recompression cycle

![Recompression cycle diagram](image)

**Figure 1.5:** Schematic of the recompression cycle PCS employed in the reference reactor [1.11]

The selected reactor thermal hydraulic design, a 2400 MW$_{th}$ S-CO$_2$ cooled fast reactor with a direct Brayton cycle with recompression, has been described in detail by M.A. Pope [1.12]. The PCS of the reactor used in this thesis was designed by V. Dostal [1.11]. Both of these contributions will be discussed briefly below as their combination defines the reference reactor employed by this thesis.). A list of selected parameters for
the S-CO₂ reactor is given in Table 1.4. Figure 1.5 shows a flow diagram for the power conversion system (PCS).

<table>
<thead>
<tr>
<th>Parameter (unit)</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal Power (MW)</td>
<td>2400</td>
</tr>
<tr>
<td>Coolant Type</td>
<td>Supercritical CO₂</td>
</tr>
<tr>
<td>Coolant Peak Pressure (MPa)</td>
<td>20</td>
</tr>
<tr>
<td>Reactor T&lt;sub&gt;in&lt;/sub&gt; (°C)</td>
<td>485.5</td>
</tr>
<tr>
<td>Reactor T&lt;sub&gt;out&lt;/sub&gt; (°C)</td>
<td>650</td>
</tr>
<tr>
<td>Power Density [kW/liter core]</td>
<td>86</td>
</tr>
<tr>
<td>q'' [kW/liter fuel]</td>
<td>151</td>
</tr>
<tr>
<td>Cycle thermal efficiency [%]</td>
<td>50.8</td>
</tr>
<tr>
<td>Specific Power [kW/kg HM]</td>
<td>20.7</td>
</tr>
<tr>
<td>PCS loops</td>
<td>4 x 25%</td>
</tr>
<tr>
<td>Cladding material</td>
<td>ODS MA956</td>
</tr>
<tr>
<td>Reflector material</td>
<td>Titanium</td>
</tr>
</tbody>
</table>

The reactor itself contains four separate power conversion loops, each circulating 25% of the coolant. In addition to the PCS loops, there are four 50% active shutdown/emergency cooling system loops for accident scenarios, although the incorporation of these loops can be omitted when a direct extraction integration method is employed for integration of the HTSE plant with the reactor, as discussed in section 3.1.2. A cartoon depicting the reference design with active SCS/ECS loops (one of four) is shown in Fig. 1.6. The turbomachinery used is extremely compact and is a single shaft design with no intercoolers. Each of the recuperators, precoolers, and the decay heat
removal heat exchangers are HEATRIC® Printed Circuit Heat Exchangers (PCHE). For further information regarding the thermal hydraulic design of the S-CO₂-GFR, refer to Ref. [1.12]. It should be noted that the GFR and the PCS are works in progress. For example, Ref. [1.11] describes the latest, 3rd generation version of the PCS.

Figure 1.6: Schematic of the S-CO₂ GFR reference design with active SCS/ECS loops (one of four depicted) [1.12]
1.5 Organization

This thesis begins by comparing several types of gas cooled reactors, detailing the specific advantages and disadvantages of each in chapter two. The reasons for selecting the S-CO$_2$-GFR are then discussed. An investigation of the different methods for integrating the S-CO$_2$-GFR reactor with the hydrogen production plant follows in chapter three. Two of the more promising designs for integration are discussed in detail, and the methods for comparing these two designs are described. Following the discussion of layout designs, the basic structure of the HTSE design is described in chapter four. The techniques used to model the electrolyzer are described, and the comparison of these modeling techniques with experimental data is also given in chapter five. The results of the numerical calculations and modeling are also included in chapter five. Finally, the results of the modeling are used to draw several conclusions. These conclusions are summarized in chapter six.
Chapter 2 Gas Cooled Reactors

The concept of a gas cooled thermal reactor is not new. Commercial gas-cooled reactors, MAGNOX followed by AGRs, have been operational in the United Kingdom since the 1960’s. Recently, several advanced designs for commercial gas cooled reactors have been developed, based upon improvements in the original gas-cooled reactor designs. [2.1] All of these commercial advanced gas-cooled reactors are thermal spectrum units. Currently, several fast spectrum designs have been proposed as well. These reactors, known as gas-cooled fast reactors (GFR), originally studied in the 1970’s have never reached the prototype stage, but are once again the focus of several studies [2.2]. In this chapter, the existing commercial thermal gas cooled reactors will be briefly discussed, followed by a description of the advanced GFR design using supercritical carbon dioxide (GFR-S-CO₂) which is the focus of the current study.

2.1 Development of Gas-Cooled Reactors

Due to the wide range of gas reactor types and designs, some attempt at an organized discussion of the development of gas cooled reactors is appropriate. As noted in Fig. 2.1, there are two basic types of gas cooled reactors: helium-cooled gas-cooled reactors, and CO₂-cooled gas-cooled reactors. Each of these basic reactor types has two subgroups: fast spectrum reactors, and thermal spectrum reactors. Each type has different advantages and disadvantages, as discussed below.
The development of thermal spectrum gas cooled reactors dates back to the 1960’s where the CO₂ cooled thermal spectrum units were first developed. Commercial reactors (British MAGNOX reactors) were built prior to this period, as described in section 2.2. In the 1970’s in addition to the thermal designs for He-cooled reactors, new designs for fast spectrum reactors were developed. These gas fast reactor (GFR) designs included the gas cooled fast reactor (GCFR) by General Atomic Co. (USA), the Gas Breeder Reactor 4 (GBR 4) by the Gas Breeder Reactor Association (EU), and the existing technology (i.e. CO₂) fast reactor (ETGBR) by CFGR (UK). Table 2.1 lists some of the characteristics of these reactors. The ETGBR was proposed as a CO₂-cooled reactor, while the other two fast reactors were proposed as He-cooled reactors. Thermal

![Figure 2.1: Taxonomic Timeline for Gas Cooled Reactors](image)
reactor development in this period consisted of the Advanced Gas Reactor (AGR) in the UK, to replace the previously run MAGNOX reactors.

<table>
<thead>
<tr>
<th>Project</th>
<th>GCFR-GA</th>
<th>GBR 4</th>
<th>ETGBR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Designer</td>
<td>General Atomic Co. (USA)</td>
<td>Gas Breeder Reactor Association (EU)</td>
<td>CEGB (UK)</td>
</tr>
<tr>
<td>Power (MWe)</td>
<td>300</td>
<td>1200</td>
<td>635</td>
</tr>
<tr>
<td>Cycle</td>
<td>Rankine</td>
<td>Rankine</td>
<td>Rankine</td>
</tr>
<tr>
<td>Coolant/Pressure (MPa)</td>
<td>He / 9</td>
<td>He / 9</td>
<td>CO₂ / 4,1</td>
</tr>
<tr>
<td>Core Flow</td>
<td>Down. Later Up</td>
<td>Upflow</td>
<td>Upflow</td>
</tr>
<tr>
<td>Core Exit T. °C</td>
<td>575</td>
<td>565</td>
<td>525</td>
</tr>
<tr>
<td>Driver Fuel</td>
<td>MOX, steel clad pins</td>
<td>MOX, steel clad pins</td>
<td>MOX, steel clad pins</td>
</tr>
<tr>
<td>Avg. Power Density kW/L</td>
<td>235</td>
<td>188</td>
<td>170</td>
</tr>
<tr>
<td>Specific Power, kW/kg HM</td>
<td>95</td>
<td>81</td>
<td>58</td>
</tr>
<tr>
<td>Pressure Vessel</td>
<td>PCRV</td>
<td>PCRV</td>
<td>PCRV</td>
</tr>
<tr>
<td>Shutdown Heat Removal</td>
<td>3 Aux. Loops Circulators &amp; Hxers</td>
<td>3 Aux. Loops Circulators &amp; Hxers</td>
<td>3 Aux. Loops Circulators &amp; Hxers</td>
</tr>
</tbody>
</table>

In the late 1970’s and throughout the 1980’s, fast spectrum reactor development stopped while several new concepts for thermal spectrum reactors were developed. These designs were limited to He-cooled reactors, and included the HTGR and the THTR reactor. Development of these reactors declined throughout the 1990’s but in the current decade, due in part to the revived interest in nuclear power, several designs for both fast spectrum and thermal spectrum reactors have surfaced for both He-cooled and CO₂ cooled reactors. Table 2.2 lists the representative contemporary closed Brayton cycle gas
turbine plant projects, underlining the trend to move away from the previously dominant Rankine cycle for gas cooled reactor power conversion systems due to the higher efficiency achievable by the Brayton cycle.

Table 2.2: Representative Contemporary Closed Brayton Cycle Gas Turbine Plant Layouts [2.3]

<table>
<thead>
<tr>
<th>Concept</th>
<th>Arrangement/Layout</th>
</tr>
</thead>
</table>
| GTHTR 300 (JAERI) | Turbine/compressor/generator encapsulated in horizontal pressure vessel  
Direct cycle: 300 MWe  
Recuperator/precooler encapsulated in separate vertical pressure vessel |
| ESKOM PBMR (South Africa) | Vertical heat exchanger vessel, connected by ducts; generator outside horizontal turbomachinery train; Direct cycle: 175 MWe |
| GRMHR (US/GA, Russia) | Vertical Pressure Vessel enclosing Turbine/HP & LP compressors in central cylinder, precooler/intercooler/recuperator in surrounding annulus; generator in vessel extension  
Direct Cycle: 285 MWe |
| MIT PBMR         | Fully dispersed among a total of 21 railcar/truck-shippable modules: e.g. six recuperator modules  
Indirect Cycle: 115 MWe |
| MIT/INL LDRD     | Single vertical PCU vessel housing all S-CO₂ components, with generator outside vessel  
Direct Cycle, Fast Reactor: 250 MWe |
| CEA              | Study of dispersed HE and S-CO₂ PCS Indirect Cycles for GFR; He primary coolant.  
Single shaft horizontal turbomachinery: 300 MWe |
| NGNP             | Both integrated and non-integrated Direct Cycle versions under consideration GTMHR used for INL Point Design studies |
| Framatome        | Indirect Cycle, N₂/He working fluid, Rankine bottom cycle: 300MWe |
| INL              | CO₂ power cycle which approaches the critical pressure (7.38 MPa) from below.  
Indirect Cycle: 125 MWe  
He, N₂/He, CO₂: 300 MWe |
| ANL              | S-CO₂ power cycle very similar to the MIT version; Indirect Cycle  
Star LM @ 180MWe |
| Tokyo Tech       | Another CO₂ power cycle which approaches the critical pressure from below; Direct Cycle; more recently S-CO₂ similar to MIT: 300 MWe |
| ORNL             | Indirect Cycle; liquid salt cooled core coupled to a helium PCS which employs multi-reheat, AHTR,  
He: 300- 1000 MWe |
| UCB              | NGNP: He, N₂/He: 300- 1000 MWe, multi-reheat |

note: designs are evolving and hence specifications change over time
2.2 Gas Cooled Thermal Reactors [2.3]

Gas cooled reactors were first built in 1955 in England. This design was known as the MAGNOX reactor, named after the magnesium alloy used as fuel. These reactors used carbon dioxide as the coolant, and graphite as the moderator, and were fueled by natural uranium. Additional gas-cooled reactors were constructed in the US, France, Spain, Switzerland, Germany, Czechoslovakia, and Italy from 1959-1973. These gas-cooled thermal reactors had net electricity generation ranging from 38-540 MWₑ, with temperatures ranging from 305-414°C. Though such reactors are no longer constructed, (only 22 of the 55 gas-cooled reactors constructed are still operational) they led directly to the British advanced gas cooled reactors (AGR) [2.4].

A sectional view of the AGR is shown in Fig. 2.2. The AGR design is similar to the MAGNOX reactor; it is graphite moderated, and gas cooled. The cladding is no longer MAGNOX, however, and a prestressed concrete reactor vessel (PCRV) lined with steel has been added for safety purposes. This vessel is gas tight, and is protected from the high temperature gas by insulation that lines the entire reactor vessel inner surface. The coolant gas is carbon dioxide with a system pressure of 4.2 MPa, and a reactor outlet temperature of around 645°C. The overall capacity of the AGR is between 555-625 MWₑ. A fuel element for this reactor consists of a 36 pin cluster of steel clad UO₂ fuel encased in graphite fuel sleeves with rods measuring 1 meter in length. In each fuel channel, 8 of these fuel elements are grouped vertically allowing on-load refueling through one pile cap standpipe provided per channel. The steam generators are inside the
PCRV, and the design of these generators follows the once through design. The power cycle for the commercial AGR is the Rankine cycle. Several stages of development occurred in the 60’s, 70’s and 80’s to improve the design of the AGR.

![Design schematic for an AGR (Heysham II/Torness A.G.R. Nuclear Island)](image)

**Figure 2.2: Design schematic for an AGR (Heysham II/Torness A.G.R. Nuclear Island)** [2.3]

Several current designs for gas-cooled reactors have been proposed and are now being studied, including the HTGR, the pebble bed modular reactor (PBMR), and other very high temperature reactors (VHTR). Though these thermal spectrum reactors are promising, the fast reactor can perform comparably, but with several additional benefits: the GFRs have the potential to close the fuel cycle, and to extend fuel resource life through their breeding capabilities. Because of these large advantages, the GFR will be the focus of this thesis.
2.3 Gas Cooled Fast Reactors

No GFRs have been constructed to date; all of the previously constructed GCRs have been thermal spectrum. There were significant GCFR development programs in the US and Europe in the 1970's, however, which included both analysis and experiments [2.3]. Most of these programs involved the use of helium coolant with the Rankine power cycle, rather than CO₂ cooled reactors and/or gas turbines. A more advanced design is being developed now for the Gen IV GFR, with several improvements. These improvements include lowering the power density from 200kW/L to 100kW/L to enhance safety, eliminating breeding blankets to avoid weapons grade plutonium production, the utilization of carbide and nitride fuels rather than oxide fuels, increasing reactor outlet temperature, the conversion to a Brayton cycle PCS, and the use of passive decay heat removal systems as far as practicable. The Gen IV GFR design has two primary variations: the MIT S-CO₂-GFR, and the mainstream He-cooled GFR.

2.3.1 CO₂-Cooled Gas-Cooled Fast Reactors

To date, the CO₂-Cooled GFR development includes three primary designs: the Existing Technology Gas-Cooled Breeder Reactor (ETGBR) [2.4], the Enhanced Gas Cooled Reactor (EGCR) [2.5], and the MIT GFR [1.11]. The ETGBR is a UK design utilizing their experience with the AGRs developed in the 1970's. It is a 1680 MWth reactor at 4.2 MPa, with outlet temperatures of 525°C. The EGCR was a BNFL and
Japanese version developed in 1998. It is a 1400 MWₑ reactor based on Heysham2/Torness AGRs. The MIT GFR design has been under development since 2000. It is the reactor design described in chapter 1, and will be the focus of this thesis.

2.3.2 Helium-Cooled Gas-Cooled Fast Reactors

Current designs for the Generation IV Gas Cooled Fast Reactor have been developed by the Commissariat à l’Energie Atomique (CEA) and the Idaho National Laboratory (INL) [2.6]. These reactors utilize a direct Helium Brayton PCS similar to the S-CO₂ PCS described in section 1.2. A schematic for the helium Cooled GFR is shown in Fig. 2.3. There are two primary designs that have been highlighted as a possible reference reactor: the 600 MWₜʰ Helium Cooled GFR, and the 2400 MWₜʰ Helium Cooled GFR [2.7]. The 600 MWₜʰ design is small enough that it is possible to make it a modular plant design (i.e. it has a small vessel, core, PCS, and other components, that would enable its direct transportation to the reactor site.) Additionally, it can utilize the 300 MW VHTR balance-of-plant (BOP) development, thus minimizing research and development costs. The 2400 MWₜʰ design has a better neutron economy, reducing the heavy metal inventory requirements per MW, it is more adaptable to a large base load operation, and it can utilize the VHTR reactor pressure vessel (RPV) size/technology (i.e., the core will fit in a current VHTR RPV) which reduces research and development
costs as well. Although the 2400 MW\textsubscript{th} design has some unique advantages, only preliminary designs for this reactor have been evaluated. Therefore, the focus of this discussion will be on the properties of the 600 MW\textsubscript{th} design.

The most attractive aspect of the helium cooled GFR is the high efficiencies involved with electricity generation. Depending on the design used, the helium cooled GFR PCS net efficiencies range from 40\% -52\%. The outlet conditions of the helium cooled GFR are 850°C and 7 MPa. As a point of reference, the thermal spectrum PBMR has reported efficiencies based upon the outlet temperature of the reactor [2.8]. This is shown in Fig. 2.4.
As with the other GFR designs, the neutronics feature a fast spectrum, and this spectrum combined with the full recycle of actinides does not produce a significant amount of long lived transuranic wastes. Other specifications for the 600 MW\textsubscript{th} reference design of the Helium Cooled GFR are listed in Table 2.3.

There are additional characteristics of a GFR that have been affirmed through the study of the reference helium cooled design. Thermal spectrum gas-cooled reactors coupled to a direct cooling cycle operate with a large assurance of safety against unprotected accidents. This property is granted by a combination of the low power density, high temperature to fuel failure, a large Doppler feedback, and a large thermal inertia. In contrast, in a GFR, the power density is an order of magnitude greater, the coolant density adds reactivity during depressurizing accidents, and there are no large blocks of graphite to provide thermal inertia. This means that the reactivity feedbacks play a much larger role in the safety of the GFR as compared to thermal spectrum gas

Figure 2.4: Plot of efficiency versus temperature for a PBMR [2.7]
Table 2.3: Parameters for the INL Helium Cooled GFR reference Design [2.7]

<table>
<thead>
<tr>
<th>System Parameter</th>
<th>Reference Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power level</td>
<td>600 MWeh</td>
</tr>
<tr>
<td>Net efficiency</td>
<td>42%</td>
</tr>
<tr>
<td>Coolant pressure</td>
<td>70 bar</td>
</tr>
<tr>
<td>Outlet coolant temperature</td>
<td>850 °C</td>
</tr>
<tr>
<td>Inlet coolant temperature</td>
<td>490 °C</td>
</tr>
<tr>
<td>Nominal flow &amp; velocity</td>
<td>330 kg/s &amp; 40 m/s</td>
</tr>
<tr>
<td>Core volume</td>
<td>11 m³ (H/D ~ 1.7/2.9 m)</td>
</tr>
<tr>
<td>Core pressure drop</td>
<td>~0.4 bar</td>
</tr>
<tr>
<td>Volume fractions of Fuel/Gap/SiC</td>
<td>50/40/10 %</td>
</tr>
<tr>
<td>Average power density</td>
<td>55 MW/m³</td>
</tr>
<tr>
<td>Reference fuel composition</td>
<td>UPuC/SiC (50/50 %)</td>
</tr>
<tr>
<td>Breeding/Burning performances</td>
<td>fissile breakeven</td>
</tr>
<tr>
<td>In core heavy metal inventory</td>
<td>30 tonnes</td>
</tr>
<tr>
<td>Fissile (TRU) enrichment</td>
<td>~20 wt%</td>
</tr>
<tr>
<td>Fuel management</td>
<td>multi-recycling</td>
</tr>
<tr>
<td>Fuel residence time</td>
<td>3 x 829 dfpd</td>
</tr>
<tr>
<td>Discharge burnup ; damage</td>
<td>~5 at%; 60 dpa</td>
</tr>
<tr>
<td>Primary vessel diameter</td>
<td>&lt;7 m</td>
</tr>
</tbody>
</table>

cooled reactors such as the AGR. To compensate for this, the primary initial engineering focus of the GFR design was to incorporate sufficient inherent negative reactivity feedback coefficients to safely adjust core power in any scenario. For a full discussion of the Helium Cooled GFR as well as the details and scheduling for the development and construction of a Helium Cooled GFR pilot plant, the reader is referred to [2.9].

2.3 Supercritical Carbon Dioxide-Cooled vs. Helium Cooled

The S-CO₂ Cooled GFR, as introduced in section 1.4, is the reactor evaluated in this thesis for nuclear hydrogen production. As with the Helium Cooled GFR reference design, the S-CO₂ Cooled GFR design with a direct Brayton cycle PCS realizes net efficiencies of around 52% when reactor outlet temperatures approach 750°C. Similar
safety concerns exist for the S-CO2-cooled reactors as for the helium-cooled reactors [1.10]. The difference, therefore, in the two reactors is small, but sufficient to warrant a discussion as to the selection of the S-CO2 reactor for the present work.

There are two primary reasons for the utilization of the S-CO2 cooled reactor design rather than the helium cooled reactor design: lower reactor outlet temperatures, and more compact turbomachinery.

2.3.1 Reactor Outlet Temperature Comparison

As can be seen in Table 2.4, there are several similar features of the two reactor types. The data for the SICO2 reactor in this comparison were provided by an in-depth analysis of optimal PCS cycles in combination with an SICO2 reactor [2.10]. This table tabulates the properties of a 300 MWc reactor cooled by S-CO2 in a direct recompression cycle, as discussed in section 1.4, as well as a helium cooled reactor.

For the same power output levels, the efficiency is almost the same for the basic one-compressor helium reactor and the S-CO2 reactor (the helium reactor is approximately 2% more efficient based on thermal efficiency - cycle efficiency not including piping, generation, or operational losses) which is reduced to negligible levels when generation and piping inefficiencies are applied. The primary differences between the conditions of these reactors are the reactor outlet temperatures and pressures. For all of the helium cooled reactors, the outlet temperature reaches or exceeds 880°C, while for
Table 2.4: Comparison of S-CO2 cooled direct recompression cycle reactor design with Helium cooled reactor design with 1 compressor (adapted from [1.11])

<table>
<thead>
<tr>
<th>Cycle type</th>
<th>S-CO2 Recompression</th>
<th>Helium 1 Compressor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power (MWₑ)</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>Turbine Inlet Temperature (°C)</td>
<td>550</td>
<td>880</td>
</tr>
<tr>
<td>Compressor Inlet Temperature (°C)</td>
<td>32</td>
<td>30</td>
</tr>
<tr>
<td>Compressor Inlet Pressure (MPa)</td>
<td>7.63</td>
<td>4.21</td>
</tr>
<tr>
<td>Compressor Outlet Pressure (MPa)</td>
<td>20</td>
<td>8</td>
</tr>
<tr>
<td>Pressure Ratio</td>
<td>2.62</td>
<td>1.9</td>
</tr>
<tr>
<td>Thermal Efficiency (%)</td>
<td>46.07</td>
<td>49.25</td>
</tr>
<tr>
<td>Thermal Power (MWₑ)</td>
<td>651.18</td>
<td>609.14</td>
</tr>
<tr>
<td>Mass Flow Ratio (kg/s)</td>
<td>3485.41</td>
<td>472.21</td>
</tr>
<tr>
<td>Volumetric Flow Rate (Turbine Inlet) (m³/s)</td>
<td>28.45</td>
<td>145.74</td>
</tr>
<tr>
<td>Heat Addition (kJ/kg)</td>
<td>186.83</td>
<td>1289.95</td>
</tr>
<tr>
<td>Turbine Work (kJ/kg)</td>
<td>122.42</td>
<td>1164.84</td>
</tr>
<tr>
<td>Compressor Work (kJ/kg)</td>
<td>36.34</td>
<td>529.54</td>
</tr>
<tr>
<td>Ratio of Compressor Work to Turbine Work</td>
<td>0.297</td>
<td>0.455</td>
</tr>
<tr>
<td>Heat Regeneration (kJ/kg)</td>
<td>516.34</td>
<td>2602.05</td>
</tr>
<tr>
<td>Turbine Work (MW)</td>
<td>426.68</td>
<td>550.05</td>
</tr>
<tr>
<td>Compressor Work (MW)</td>
<td>126.68</td>
<td>250.05</td>
</tr>
<tr>
<td>Heat Regeneration (MW)</td>
<td>1799.66</td>
<td>1228.71</td>
</tr>
<tr>
<td>Precooler Inlet Temperature (°C)</td>
<td>70.75</td>
<td>156.13</td>
</tr>
<tr>
<td>Temperature Rise Across the Core (°C)</td>
<td>151.67</td>
<td>248.66</td>
</tr>
</tbody>
</table>

The S-CO₂ reactor the outlet temperature is 550°C to 650°C. The helium cooled reactor outlet temperature is so high that it poses serious challenges for materials selection in the reactor, making it a potentially less desirable option. The S-CO₂ reactor outlet temperature, however, is low enough that significant material selection challenges do not occur. The pressure for the S-CO₂ reactor is 20 MPa, much higher than the helium
reactor's 8 MPa. This, however, is tolerable and less than the contemporary supercritical Rankine power cycle practice in which 25 MPa and higher is employed. Finally, three decades of AGR experience at 650°C have provided a large database for CO\textsubscript{2} plant performance upon which the CO\textsubscript{2} GFR can build with considerable confidence.

2.3.2 Turbomachinery Comparison

A second major advantage to the S-CO\textsubscript{2} reactor is the compact nature of the cycle spatially. The mass flow rate of coolant in the S-CO\textsubscript{2} reactor is more than that in the helium reactor by a factor of nearly ten. However, the volumetric flow rate is nearly five times less for the S-CO\textsubscript{2} reactor than for the helium reactor. These numbers serve to indicate how dense the supercritical carbon dioxide is in comparison with the helium. Because the density of supercritical carbon dioxide is so high (nearly as high as water at lower temperatures) the equipment need not be as large as it is for a less dense coolant like helium. Supercritical CO\textsubscript{2} turbomachinery, particularly the turbine, in the PCS cycle will be much more compact, and in return the capital costs of the PCS will be reduced [1.11]. In addition, a supercritical carbon dioxide turbine is significantly smaller than steam turbines. Because of the compact nature of the S-CO\textsubscript{2} turbomachinery, this reactor design is superior to Rankine Cycle designs. For a complete discussion refer to [2.11]
2.4 Gas-Cooled Reactor Summary

S-CO₂ Gas reactors have been used for commercial power generation in the UK for nearly 30 years, however coupled to Rankine based turbine plants. Experience operating these thermal reactors has led to the development of advanced gas reactors which can operate at higher temperatures, and are more efficient than the earlier MAGNOX designs. Fourteen of these thermal spectrum AGR designs are still in operation today. Experience gained in operating these AGRs has led to the development of even more advanced thermal gas reactors but with helium as a coolant, including the GT-MHR, the PBMR, and the VHTR. These designs vary widely, including both He and CO₂ cooled concepts. Additionally, some fast spectrum advanced gas reactor designs have been developed for potential use. Two GFR designs are being considered for future construction. The first design is the helium-cooled GFR. This design is currently the reference design for the Generation IV GFR. The second design is the supercritical carbon dioxide-cooled GFR, as described in this paper. Though both are highly advanced with very high efficiencies, the S-CO₂ reactor is employed in this paper as the reactor of choice for hydrogen generation purposes as it has a lower reactor outlet temperature, which eliminates the need for expensive high temperature material requirements, and for its spatially compact design. The reader should keep in mind, however, that because both reactors have comparable thermodynamic efficiencies, both reactors are viable options for use in hydrogen production by electrolysis, as are other reactors that can deliver high electricity generation efficiently.
Chapter 3 Hydrogen Production Plant

There are several methods proposed for nuclear hydrogen production. However, this work focuses on high temperature steam electrolysis (HTSE). This method uses nuclear heat to raise steam to high temperatures, and uses nuclear electricity to split the steam into hydrogen and oxygen using a high temperature electrolyzer. This requires both thermal and electrical energy. The thermal energy is provided by part of the supercritical carbon dioxide (S-CO$_2$) coolant directly in a water boiler loop, while the electrical energy is provided by the PCS of the GFR.

3.1 Description of the HTSE plant

A nuclear hydrogen plant should minimize the total external heat input required, so that the efficiency is maximized. This can be accomplished by ensuring that the heat recuperation of the system is maximized. The following analysis follows a similar approach to a study performed by Yildiz, Hohnholt, and Kazimi to this effect [3.2]. A layout of an HTSE plant is given in Fig. 3.1. In this layout, there are two primary sources of heat: heat from the GFR-S-CO$_2$ reactor, and heat from product gases. The heat from the GFR-S-CO$_2$ reactor serves to create supersaturated steam from the process feedwater. There are several possibilities for extracting this heat from the reactor; two of the most promising of which are discussed later in this work. Heat recuperation in the HTSE plant is divided into two segments: oxygen recuperation and hydrogen recuperation. The
oxygen recuperation occurs in the exchanger $R_O$ while the hydrogen recuperation occurs in the exchanger $R_H$. The heat from each of these product streams is used to heat the steam to just below the required HTSE levels, about 870 °C. The temperatures of each of these streams (indicated by the numbers in Figure 3.1) are given in Table 3.1 while the split ratio of the steam, based upon the heat capacity of the product gases at the given pressures, is given in Table 3.2.
Table 3.1: HTSE flow stream temperatures at different locations for three different operating pressures

<table>
<thead>
<tr>
<th>Point</th>
<th>P=0.1MPa Temperature (°C)</th>
<th>P=3MPa Temperature (°C)</th>
<th>P=7MPa Temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>30.0</td>
<td>30.0</td>
<td>30.0</td>
</tr>
<tr>
<td>2</td>
<td>100.0</td>
<td>233.9</td>
<td>278.2</td>
</tr>
<tr>
<td>2a</td>
<td>100.0</td>
<td>233.9</td>
<td>278.2</td>
</tr>
<tr>
<td>2b</td>
<td>100.0</td>
<td>233.9</td>
<td>278.2</td>
</tr>
<tr>
<td>3a</td>
<td>870.0</td>
<td>870.0</td>
<td>870.0</td>
</tr>
<tr>
<td>3b</td>
<td>870.0</td>
<td>870.0</td>
<td>870.0</td>
</tr>
<tr>
<td>4</td>
<td>900.0</td>
<td>900.0</td>
<td>900.0</td>
</tr>
<tr>
<td>5</td>
<td>900.0</td>
<td>900.0</td>
<td>900.0</td>
</tr>
<tr>
<td>6</td>
<td>265.8</td>
<td>345.7</td>
<td>346.2</td>
</tr>
<tr>
<td>7</td>
<td>900.0</td>
<td>900.0</td>
<td>900.0</td>
</tr>
<tr>
<td>8</td>
<td>265.8</td>
<td>345.7</td>
<td>346.2</td>
</tr>
</tbody>
</table>

Table 3.2: Flow split ratios of H₂O before product stream heat exchangers

<table>
<thead>
<tr>
<th>% of flow in</th>
<th>P=0.1MPa</th>
<th>P=3MPa</th>
<th>P=7MPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream a</td>
<td>36.3</td>
<td>36.5</td>
<td>36.6</td>
</tr>
<tr>
<td>Stream b</td>
<td>63.7</td>
<td>63.5</td>
<td>63.4</td>
</tr>
</tbody>
</table>

3.2 Integration of the HTSE plant

The integration of a hydrogen production facility with a nuclear GFR- S-CO₂ should optimize the overall hydrogen production process efficiency (η_H₂), but for an effective integrated system, other aspects must be optimized as well. Areas which merit a closer investigation include physical limitations, thermal hydraulic influences, thermodynamic effects, and safety issues. If the maximum hydrogen production process
efficiency comes at the detriment of one of the other areas, a less efficient design may be desired. Several methods for integrating the HTSE unit with a S-CO₂ GFR have been modeled to determine the optimal method of integration. This integration involves the extraction of heat from the current reactor electricity-only generation cycle to heat the pre-heated water in the primary boiler of the HTSE plant. These methods include systems which extract heat from the reactor from several different points:

1. Extraction of heat from the Power Conversion System (PCS) turbine exhaust
2. Extraction of heat from the PCS immediately following the high temperature recuperator
3. Extraction of heat immediately following the low temperature recuperator
4. Extraction of heat from pre-cooler
5. Extraction of heat directly from the reactor using separate water boiler loops

A summary of the designs along with their respective shortcomings or advantages is given in Fig. 3.2.

Two of the designs that were modeled have been found to be the most promising methods for integrating the HTSE unit with an S-CO₂-GFR. The first method of integration is to extract S-CO₂ directly from PCS after a stage or more of turbine expansion. The second method of integration is the extraction of S-CO₂ directly from the reactor itself, resulting in completely separate loops dedicated to the HTSE plant. The two post-recuperator methods produce steam at temperatures at which the vapor pressure is too low to provide the pressure suitable for pumping the hydrogen (~3-5 MPa), while the pre-cooler is at such a low temperature that it cannot boil the feedwater.
<table>
<thead>
<tr>
<th>Schematic of method</th>
<th>Description of method</th>
<th>Primary Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Diagram" /></td>
<td>Extraction of heat from turbine exhaust of PCS</td>
<td>Low thermodynamic efficiency loss with low capital costs</td>
</tr>
<tr>
<td><img src="image" alt="Diagram" /></td>
<td>Extraction of heat immediately after the high temperature recuperator</td>
<td>Steam temperature too low to maintain pumping pressure of hydrogen</td>
</tr>
<tr>
<td><img src="image" alt="Diagram" /></td>
<td>Extraction of heat immediately after the low temperature recuperator</td>
<td>Steam temperature too low to maintain pumping pressure of hydrogen</td>
</tr>
<tr>
<td><img src="image" alt="Diagram" /></td>
<td>Extraction of heat directly from reactor using separate water boiler loops</td>
<td>Low thermodynamic efficiency loss with safety benefits arising from separate cooling loops</td>
</tr>
<tr>
<td><img src="image" alt="Diagram" /></td>
<td>Extraction of heat from the precooling unit</td>
<td>Heat quality not sufficient to boil feed water</td>
</tr>
</tbody>
</table>

**Figure 3.2:** Summary of HTSE/GFR integration designs modeled
3.2.1 Extraction of S-CO$_2$ from Power Conversion System (PCS) Turbine Exhaust

Yildiz, Hohnholt, and Kazimi have analyzed the method of extracting SCO$_2$ from the PCS directly [3.2]. A depiction of such a layout is given in Figure 3.3. This method allows for the extraction of S-CO$_2$ immediately after the PCS-S-CO$_2$ turbine. This S-CO$_2$ is then used to boil the water in the intermediate heat exchanger (IHX). Due to significant pressure losses in the IHX, the S-CO$_2$ is subsequently compressed, and returned to the PCS by insertion into the hot side of the high temperature recuperator.

There are several advantages for the extraction of the S-CO$_2$ directly from the turbine exit. The first is that the IHX cost is reduced. The inlet for the hot side of an IHX fed directly by coolant from the reactor in the separate WB loops design could experience temperatures between 550°C and 750°C. The hot side pressure is approximately 20 MPa. The cold side inlet temperature is approximately 32°C, and the pressure ranges from atmospheric pressure to 7 MPa.
Figure 3.3: Schematic showing Schematic I of an integrated HTSE-S-CO₂-GFR plant: coolant extracted directly from the PCS, with recuperation of heat into the steam from the hydrogen and oxygen product streams.

These high temperature and pressure differentials greatly restrict the materials selection for the IHX. Materials must be durable, and able to withstand such differentials, but such materials can be costly. The design shown in Figure 3.3 allows for greater flexibility in selecting materials, as the hot side inlet temperature and pressure are both reduced. Table 3.3 shows the IHX inlet conditions for each design.

The second advantage is that thermodynamic efficiency for the nuclear electricity production in this design is slightly higher than for separate WB loops. Table 3.4 compares the electrical thermodynamic efficiencies for both processes, or the ratio of the electrical energy produced to the thermal energy required to produce that amount of
electricity, of the PCS loop for each of the designs. This comparison was made at three different reactor outlet temperatures: the lowest, 550°C reflects the conditions for current reactor technologies, 650°C represents reactor outlet temperatures for near future technological advancements, while the highest temperature, 750°C is the hoped for outlet temperature after long term technological advancements in reactor design and materials science. Overall, the efficiency tends to be greater in the direct extraction design, but only by a fraction of a percent, which is not a significant amount.

Table 3.3: IHX inlet conditions for heat extraction from PCS and for separate water boiler loops

<table>
<thead>
<tr>
<th></th>
<th>Low T (°C)</th>
<th>High T (°C)</th>
<th>Pressure (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCS Extraction (Turbine outlet)</td>
<td>445</td>
<td>630</td>
<td>8</td>
</tr>
<tr>
<td>Separate WB Loops (Direct from Reactor)</td>
<td>550</td>
<td>750</td>
<td>20</td>
</tr>
</tbody>
</table>

Table 3.4: PCS Thermodynamic efficiencies for electricity generation for coolant extraction from PCS and for separate water boiler loops for three different reactor outlet temperatures

<table>
<thead>
<tr>
<th></th>
<th>550 (°C)</th>
<th>650 (°C)</th>
<th>750 (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCS Extraction (Turbine exhaust)</td>
<td>39.45%</td>
<td>42.69%</td>
<td>45.30%</td>
</tr>
<tr>
<td>Separate WB Loops (Direct from Reactor)</td>
<td>39.31%</td>
<td>42.54%</td>
<td>45.21%</td>
</tr>
</tbody>
</table>

The third advantage of this approach to the integration of the HTSE plant is the simplicity of implementation and lower capital costs. This technique requires only simple adaptations of flow and piping into and out of already present PCS units, such as
the S-CO₂ turbine, and the high temperature recuperator. The separate WB loops, however, require the implementation of new trains within the reactor vessel itself. This may include altering an already established design for the GFR, with potentially problematic consequences. This can be avoided by utilizing the direct PCS extraction layout.

The major disadvantage of this integration method is the problem of interfering with the PCS main role: electricity production. Several problems ensue when the feed temperatures and pressures of the power conversion loops are altered, particularly in the region of the recuperators, which are extremely sensitive to temperature changes. The extraction and subsequent reentry of the coolant has potentially negative influences on the operation, control, and transient response of the electricity production of the PCS. This problem is avoided with the implementation of the separate WB loops integration method.

3.2.2 Separate WB Loops [3.3]

A design for extraction of heat directly from the reactor has been created. This layout is depicted in Figure 3.4. The primary difference between Figure 3.3 and Figure 3.4 is the method for the extraction of coolant. In the separate water boiler (WB)
Figure 3.4: Schematic showing Schematic II of an integrated HTSE-S-CO$_2$-GFR plant: extraction of heat from separate WB loops in the reactor with recuperation of heat into the steam from the hydrogen and oxygen product streams.

Extraction layout, about 9.2% of the S-CO$_2$ is extracted directly from the reactor using four WB loops. These loops are completely independent of the reactor PCS, and therefore avoid the problem of tampering with the thermodynamics of the PCS. In addition, this design includes a steam turbine, which generates sufficient power to circulate the HTSE feed loops, ensuring that the HTSE plant is completely separated from the PCS. Figure 3.5 shows the principal features of the design: (one of) four parallel identical self-powered loops, each removing about 2.3 percent of the reactor's thermal power. The stream discharged from the loop's high pressure turbine normally flows to the HTSE cell via...
Figure 3.5: HTSE Water Boiler Loop (one of four) which also serves for decay heat removal

recuperators which recover thermal energy from the product hydrogen and oxygen gases.

This allows the cell to operate at a higher temperature than the reactor, and it is
maintained by ohmic heating produced by the electricity supplied by the reactor's large power conversion loops (consuming about 91% of the core thermal power): \( \text{S-CO}_2 \) Brayton units in our GFR concept [3.4]. In normal operation, and most shutdown scenarios, the turbine drives the S-CO\(_2\) loop circulator, and generates excess electricity for plant or emergency system use. The reversible motor generator can also power the blower using on-site or off-site emergency electric power.

This arrangement has several advantageous features:

1. No changes are required in the main PCS loops used to provide electricity to the HTSE cells.
2. The water boiler (WB) loops eliminate the need for separate shutdown and emergency cooling loops.
3. The WB loops are always on, which increases the probability that they will be available for SCS/ECS service. (no fail-to-start sequences, and constant diagnostic signals.)
4. The WB loops are oversized for SCS/ECS service: they are designed to remove a total of about 8.8% of core full power (2.3% each), whereas only 2% is needed for decay heat removal. The required total water boiler energy rating is such that for their use in SCS/ECS service one can have four 100% capable loops, versus the four 50% shutdown cooling system loops specified in the current all-electric design.
5. The use of four parallel trains is also desirable for their primary function of providing uninterrupted steam to the HTSE cells: one would like to have the
ability to have one loop down for maintenance and also be able to accommodate random failure in another.

6. Oversizing also facilitates operation in a passive, natural-convection-only mode, in the event that full power not be available for WB loop circulators. The steam generators also have a generous inventory of water, which relaxes the time deadline for restoration of feedwater flow.

7. Steam in the SCS/ECS mode can be vented or used to power a small turbine-generator for provision of emergency electric power (e.g., the reversible motor generator in Fig. 3.4). Steam storage accumulators can also serve both the HTSE plant and reactor emergency power turbines.

8. No adaptation of the PCS is required, reducing the probability that detrimental effects due to process changes occurs. This also limits the analysis required to determine complex effects and changing process conditions due to the extraction of S-CO$_2$ from the PCS directly.

On the negative side, this design requires modification of the reactor vessel and the extra-vessel plant layout, as the four separate WB loops need to be included in the original design. In addition, the inclusion of the steam turbine and the three additional heat exchangers will probably increase the capital costs by more than that saved by replacement of the conventional SCS/ECS loops, and certainly more than the added components in the turbine exhaust approach. Additional comparisons between the two different layouts, including thermodynamic calculations, will be conducted in Chapter 5.
3.2.2 Extraction of Heat from Low Temperature Recuperator (LTR) and Turbine Exhaust

The methods for integration of the HTSE and the GFR described in this thesis are not exhaustive. An additional method for extracting heat from the PCS of the GFR is possible, which is more thermodynamically appealing than the options modeled in this work. This method involves extracting heat in part from the LTR, and in part from the turbine exhaust as described in chapter 3.2. In other words, half of the LTR can be replaced with the IHX. This method of extracting heat from both the LTR and the turbine exhaust reduces the amount of high temperature heat extracted heat from the PCS of the GFR to boil water, while simultaneously producing steam at a sufficient temperature to provide the necessary pumping pressure (~5 MPa) for hydrogen. Future studies will need to focus on this method of integration, as it may prove to be more efficient than those methods described in chapters 3.2.1 and 3.2.2. It may also require a significantly different GFR PCS, as the properties of the recuperators will be altered due to the additional heat extraction.

3.3 Energy Balances of Plant Components

The thermodynamic properties of each layout can be used to fully analyze which one would be best for the production of nuclear hydrogen. This thermodynamic analysis requires that the energy balances of each of the plant components be derived, as done, for example, by Yildiz, Hohnholt, and Kazimi [3.2]. The derivations for the major
components common to each unit are given below, while the actual numerical calculations for each component are discussed in Chapter 5.

Heat Exchangers

Each of the several heat exchangers in the HTSE plant layout is governed by a simple energy balance, where we define the control volume to be the heat exchanger in question:

\[ E_{in} - E_{out} = E_{acc} \]  \hspace{1cm} (3.1)

Where:
- \( E_{in} \) = energy entering the control volume (kJ)
- \( E_{out} \) = energy exiting the control volume (kJ)
- \( E_{acc} \) = energy accumulated in the control volume (kJ)

Because we are performing a steady state thermodynamic comparison of the two layouts, the energy accumulation is zero. This leaves us with the following equation:

\[ E_{in} - E_{out} = 0 \hspace{1cm} \text{or} \hspace{1cm} E_{in} = E_{out} \]  \hspace{1cm} (3.2)

For any fluid flow, the energy in the stream is simply the product of the mass flow rate and the specific enthalpy, as seen in the following equation:

\[ E = m \times h \]  \hspace{1cm} (3.3)
Because conservation of mass applies, the transfer of energy in any exchanger can therefore be determined by finding the difference in enthalpy of either the hot side exchanger fluid, or the cold side exchanger fluid:

\[ Q = m \times (h_{\text{in}} - h_{\text{out}}) \]  

(3.4)

The enthalpy change for both sides will be equal so long as (3.2) applies to the exchanger:

\[ m_{\text{hot}} \times (h_{\text{hot,in}} - h_{\text{hot,out}}) = m_{\text{cold}} \times (h_{\text{cold,in}} - h_{\text{cold,out}}) \]  

(3.5)

Where:
- \( m \) = mass flow rate of fluid (kg)
- \( h_{\text{in}} \) = enthalpy of the fluid at the exchanger inlet (kJ/kg)
- \( h_{\text{out}} \) = enthalpy of the fluid at the exchanger outlet (kJ/kg)
- hot/cold subscript = indication of the hot or cold side mass and enthalpy

This equation is sufficient for the exchangers involving substances where enthalpies are carefully tabulated as a function of temperature and pressure (e.g. water, due to accessibility and accuracy of steam tables). For species where this data is not well defined, it is also acceptable to substitute an expression for the enthalpy based on the specific heat and temperature of the material, if the specific heat is fairly constant with respect to temperature:

\[ Q = C_p \times m \times (T_{\text{in}} - T_{\text{out}}) \]  

(3.6)

Where:
$T_{in} =$ temperature of the fluid at the inlet (°C)
$T_{out} =$ temperature of the fluid at the outlet (°C)
$C_p =$ Constant pressure heat capacity of the fluid. (kJ/kg*°C)

This relation is especially suitable for substances with well tabulated heat capacities, or

![Graph showing constant pressure heat capacities of various substances](image)

**Figure 3.6:** Constant pressure heat capacities (20 MPa) of various substances as a function of temperature derived from an equation of state

substances with a simple equation of state that gives the heat capacity as a function of temperature and pressure. A graph of such an equation of state for several different species is given in Fig. 3.5 which lists the temperature dependence of heat capacity for several different components at constant pressure. Either of the above methods is valid, and the selection of which equation to utilize depends on whether or not the constant pressure heat capacity is constant as temperature changes. If the heat capacity is not constant, enthalpy tables must be used instead.
If several exchangers in series are used, then equation (3.3) can be summed over each exchanger to give the following relation:

\[ Q = \sum_{i} m_i \cdot C_p_i \cdot (T_{i,\text{in}} - T_{i,\text{out}}) \]  

(3.7)

where the subscript \( i \) refers to the "ith heat exchanger, which can be used to determine the overall heat transfer rate of the exchangers.

**Reactor**

Following a similar derivation as for the heat exchangers, the heat generated in the nuclear reactor, or the heat transferred to the coolant in the reactor, is found to be equal to the increase in thermal energy of the S-CO\(_2\) coolant. This can be used by determining the change in temperature of the S-CO\(_2\) as given below:

\[ Q_R = m_{\text{CO}_2} \cdot (h_{\text{in}} - h_{\text{out}}) \]  

(3.8)

Where:

- \( Q_R \) = heat of the reactor (kJ)
- \( h_{\text{out}} \) = enthalpy of reactor outlet stream (kJ/kg)
- \( h_{\text{in}} \) = enthalpy of reactor inlet stream (kJ/kg)
- \( m_{\text{CO}_2} \) = mass flow rate of S-CO\(_2\) (kg)

**Water Boiler**
The energy required for the water boiler can be found by adding together the latent heat and the specific heat required to bring the water to the desired state. The actual heat required to boil the water is quite similar to equation (3.4), except that both the steam state and the water state must be included. The latent heat is merely the heat of vaporization of water, which can be easily found in most steam tables. The resulting equation which gives the energy required is:

\[
Q = \int_{T_{\text{win}}}^{T_{\text{sat}}} C_p(T) dT + h_{fg} + \int_{T_{\text{sat}}}^{T_{\text{super}}} C_p(T) dT
\]  

(3.9)

Where:
- \(h_{fg}\) = heat of vaporization of water (kJ)
- \(T_{\text{sat}}\) = saturation temperature of water at given pressure (°C)
- \(T_{\text{win}}\) = inlet temperature of water (°C)
- \(T_{\text{sat}}\) = saturation temperature of steam at given pressure(°C)

**Pumps/Compressors**

For an ideal pump/compressor, the work can be determined by a similar energy balance approach as for exchangers. This ideal work is determined by the following relation:

\[
W_p = m \ast (h_{p,\text{out,s}} - h_{p,\text{in}}) \quad \text{or} \quad W_c = m \ast (h_{c,\text{out,s}} - h_{c,\text{in}})
\]

(3.9, 3.10)

Where:
- \(W_p\) = work of the pump (kJ)
- \(W_c\) = work of the compressor (kJ)
- \(h_{p,\text{out,s}}\) = ideal (no entropic losses) pump outlet fluid enthalpy (kJ/kg)
- \(h_{c,\text{out,s}}\) = ideal (no entropic losses) compressor outlet fluid enthalpy (kJ/kg)
- \(h_{p,\text{in}}\) = pump fluid inlet enthalpy (kJ/kg)
- \(h_{c,\text{in}}\) = compressor fluid inlet enthalpy (kJ/kg)
For the realistic work done by a pump or compressor, the efficiency of the pump (\(\eta_p\)) or compressor (\(\eta_c\)) needs to be known (this value is readily obtained from the manufacturer of the pump or compressor), and used to determine the amount of energy lost to entropic gains. Thus, the realistic work for the pumps is actually given by

\[
W_p = \frac{W_{p,\text{ideal}}}{\eta_p} = \frac{m*(h_{p,\text{out},s} - h_{p,\text{in}})}{\eta_p} \tag{3.11}
\]

And for compressors is given by:

\[
W_c = \frac{W_{c,\text{ideal}}}{\eta_c} = \frac{m*(h_{c,\text{out},s} - h_{c,\text{in}})}{\eta_c} = \frac{1}{\eta_c} \cdot m^* R^* T_{\text{in}} * \left( \frac{k}{k-1} \right) \left( \frac{P_{\text{out}}}{P_{\text{in}}} \right)^{\frac{k-1}{k}} - 1 \tag{3.12}
\]

Where:
- \(W_{p,\text{ideal}}\) = minimum (no entropy) work required to pump a fluid to higher pressure (kJ)
- \(W_{c,\text{ideal}}\) = minimum work required to isentropically compress a fluid (kJ)
- \(k\) = ratio of constant pressure to constant volume heat capacities = \(C_p/C_v\)

**HTSE Unit**

The electrical energy required to actually electrolyze steam in the HTSE unit is in reality greater than the energy required to split steam at the process conditions. Yildiz, Hohnholt, and Kazimi have previously attempted to model this loss using an overpotential model. However, more accurate modeling of the energy required for the HTSE unit has been accomplished at the Idaho National Lab (INL) [3.4]. This work utilizes the overpotential model as an approximation of the electrical energy required; a description of the INL models will be undertaken in Chapter 4.2.2 and 4.3.3. The excess
energy, or the overpotential, is required due to certain electrical energy losses, including activation of intermediate electrolysis steps, species transfer limitations, and electrical and ohmic resistances. Thus a simple expression for the electrical work required by the HTSE unit \( (W_e) \) is given by the following equation:

\[
W_e = \Delta G_e + W_{ir}
\]  

(3.13)

where:
- \( \Delta G_e \) = Gibbs free energy for the electrolysis (kJ)
- \( W_{ir} \) = additional work required to compensate for the irreversibilities (kJ)

The overall hydrogen production energy efficiency can be determined, therefore, by noting that efficiency is equal to the ratio of energy derived from a system, to energy required by a system. To determine energy output, the lower heating value (LHV) of hydrogen was used. This value corresponds to the energy derived from a hydrogen combustion reaction in which all the product water is in liquid form. The overall process hydrogen efficiency (\( \eta_{H_p} \)), therefore, is equal to:

\[
\eta_{H_p} = \frac{\Delta G_{r,H_2}}{Q_{R,e} + \frac{\Delta G_e + W_{ir}}{\eta_{S-CO_2}}}
\]  

(3.14)

Where:
- \( \Delta G_{r,H_2} \) = Lower heating value of Hydrogen, equivalent to product energy (kJ)
- \( \eta_{S-CO_2} \) = efficiency of S-CO2-PCS system
- \( Q_{Re} \) = Thermal energy produced by reactor used to heat steam for electrolysis
This efficiency value is generally used as a point of comparison between various methods for hydrogen production, and has been used in this chapter as a means of comparing the two different HTSE plant layouts. The overall thermal to hydrogen energy conversion efficiency of the nuclear hydrogen production plant can be determined by the equation:

\[
\eta_{H_p} = \frac{\Delta G_{r,H_2}}{Q_{R,e} + \frac{\Delta G_e + W_r + W_p + W_c}{\eta_{S-CO_2}}} 
\]

(3.15)

This concludes the investigation of energy balances for individual plant components, as well as plant hydrogen production efficiency. These balances are utilized by ASPEN, a widely employed chemical process design code [3.6]. The results of these balances as performed by ASPEN are discussed in chapter 5.

### 3.4 Maximization of Thermal Recuperation

One of the most beneficial aspects of the HTSE plant design in question is the capacity to recuperate product heat to reduce the overall energy load on the system. As shown in Fig. 3.1 this recuperation is required to obtain process temperatures in the HTSE, since these temperatures are actually hotter than the reactor outlet temperatures. Maximization of this thermal recuperation is one of the primary objectives of this work. Many efforts have been made to recover as much thermal energy as possible, increasing the process efficiency for hydrogen production [3.7][3.8]. In this work, this recuperation is maximized using ASPEN.
Three techniques must be used in order to maximize thermal recuperation of water for both HTSE plant designs discussed in this work:

1. Adjust the ratio of steam flow for the flow split indicated in figure 3.1 to fully recuperate the thermal energy of both the hydrogen and oxygen product streams.

2. Reserve highest quality heat for use in high temperature applications, while maintaining lower quality heat for low temperature boiling and heating.

3. Utilize ALL excess thermal energy that is reasonable to heat streams that require heating at lower temperatures.

The implementation of these three techniques increases the thermal efficiencies to the optimized values listed in Table 3.4 (for a steam flow split of 36.35%).

The first technique compensates for the differing heat capacities of Oxygen and Hydrogen. Since both products leave the HTSE at the process temperature (900°C), but have differing heat capacities, a 50-50 split of steam flow at point 2 is highly ineffective. In addition, because there is only limited thermal energy in each product, there are physical constraints which govern the flow split ratio as well. If the amount of flow which proceeds to the oxygen recuperator is greater than 39.05% of the total flow, there will not be enough thermal energy in the oxygen to heat the steam in the oxygen recuperator to the required temperature of 870°C. Additionally, if the fraction of steam flow to the oxygen recuperator is reduced to less than 32% of the total steam flow (about 1786 kg/s), there will not be enough thermal energy in the hydrogen to heat the steam in the hydrogen recuperator to 870°C.
Fig. 3.7: Change in temperature for oxygen and hydrogen streams in the recuperator as a function of the flow split ratio: endpoints of each line indicates entrance into region of physical impossibility, while the optimal flow split ratio is indicated by the intersection of the two lines.

To determine the optimal flow split ratio, the overall heat (enthalpy) required to raise the temperature of the steam in branches 2a and 2b to 870°C was calculated as a function of the flow split ratio, and was subtracted from the available enthalpy of the hydrogen and oxygen streams respectively. (The available enthalpy here is defined as the enthalpy of the product streams at HTSE conditions, 900°C and 6MPa, less the enthalpy of the product streams after the respective recuperators.) The range in which this value for both streams is positive is the range in which the flow split is valid physically. To further reduce thermal losses through piping and fixtures, the temperature of both product
streams should be minimized as well. This will occur when the recuperator outlet streams of both the hydrogen and oxygen streams are at the same temperature. Hence the required enthalpies of the hydrogen and oxygen streams are divided by their heat capacities and their mass flow rates to give the change in temperature for each stream. Since each stream starts at the same temperature, a similar temperature drop indicates a similar temperature. The temperature change is thus plotted for each stream as a function of the flow rate, as shown in Fig. 3.7, and the intersection of these lines indicates the optimal flow split ratio for the steam. Table 3.5 gives the properties, including flow percentage, for streams 2a and 2b when the heat recuperation is maximized. The temperatures indicated were found using the ASPEN model, and are constrained by a desire to maintain a suitable vapor pressure for the steam and by heat exchanger limitations.

**Table 3.5: Properties of flow streams 2a, 2b, 6, and 8 for optimal flow split ratio**

<table>
<thead>
<tr>
<th>Stream</th>
<th>2a</th>
<th>2b</th>
<th>6</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Species</td>
<td>Steam</td>
<td>Steam</td>
<td>Oxygen</td>
<td>Hydrogen</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>196.5</td>
<td>196.5</td>
<td>249</td>
<td>249</td>
</tr>
<tr>
<td>Pressure (MPa)</td>
<td>6</td>
<td>6</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/sec)</td>
<td>33.806</td>
<td>59.194</td>
<td>10.407</td>
<td>82.593</td>
</tr>
<tr>
<td>Flow Ratio (%)</td>
<td>36.35</td>
<td>63.65</td>
<td>11.19</td>
<td>88.81</td>
</tr>
</tbody>
</table>

An additional technique for maximizing heat output is to utilize the highest quality heat for the highest temperature ranges. There are two primary purposes for selecting appropriate heat qualities for thermal recuperation. First, this will ensure that a "pinch-point" in the heat exchanger won't be reached. A pinch point occurs in a
configuration of heat exchangers in which thermodynamically, it is impossible for any further heat to be transferred across a boundary between two substances. An example of a pinch point is given in Fig. 3.8 in which a concurrent flow heat exchanger is portrayed. The CO₂ in this exchanger, though it has enough thermal energy to increase the water to a higher temperature in a different configuration, can only increase the steam temperature to about 145°C due to a physical limitation rooted in the second law of thermodynamics. This limitation, which is known as a pinch point, can be avoided if higher heat qualities are reserved for the higher temperature exchanges. Ensuring that the high quality heat

![Diagram of heat exchanger configuration](image)

**Figure 3.8: A concurrent flow heat exchanger configuration in which the transfer of heat is limited due to a “pinch-point”**

is reserved for the highest temperature applications also reduces cost and increases thermal efficiencies further. The higher quality heat is much more expensive to produce, and using it for low temperature heating, or boiling at ambient conditions, is a waste of heat that can be used at higher temperatures. By adopting this strategy and seeking to
employ the third technique of recovering all possible waste heats, an optimal design for
the HTSE layout was derived.

The final designs for the HTSE are shown in Fig. 3.9 and Fig. 3.10. These diagrams
represent the HTSE plant layout where thermal recovery has been maximized for the
direct extraction and the separate WB loops designs, respectively. As seen in both
designs, this includes additional exchangers known as the "pre-heaters". The hydrogen
and oxygen product streams after being pumped through the recuperators, still have some
excess thermal energy, as seen in Table 3.6. This energy is recuperated as low quality
heat to pre-heat the feedwater to a nearly saturated liquid. This greatly enhances the

Figure 3.9: Schematic showing Schematic I of an integrated HTSE-S-CO₂-GFR
plant: coolant extracted directly from the PCS, with optimal thermal
recuperation including preheaters and hydrogen & oxygen
recuperators
overall performance of the IHX; the feedwater can be boiled with minimal heat being utilized to heat the liquid to the saturation point. The results of this final recuperation of heat can also be seen in Table 3.6. The “With Preheater” columns indicate the final

Figure 3.10: Schematic showing Schematic II of an integrated HTSE-S-CO₂-GFR plant: extraction of heat from separate WB loops in the reactor with optimal thermal recuperation including preheater hydrogen and oxygen recuperators

hydrogen, oxygen, and feedwater stream conditions in the layout indicated in Fig. 3.9, while the “Without Preheater” columns indicate stream properties before the preheaters have been added to the system. It can be seen from this table that the heat required from the reactor is reduced by 10% when a preheater is added to the layout, utilizing the
remaining heat of the hydrogen and oxygen product streams. It should be noted that previous designs have reversed the heating order of the feedwater, heating first with the product streams, and secondly with the reactor [3.7]. This method is not recommended, however, as a pinch-point is reached at less than 650°C, and no further heating is possible without providing additional energy.

Table 3.6: Product stream properties for hydrogen, oxygen, and feedwater before and after the addition of feedwater preheating and the reactor thermal energy requirement for each system

<table>
<thead>
<tr>
<th>Stream</th>
<th>Without Preheaters</th>
<th>With Preheater</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>H₂</td>
<td>O₂</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>196.5</td>
<td>196.5</td>
</tr>
<tr>
<td>Pressure (MPa)</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>Mass Flow (kg/sec)</td>
<td>10.41</td>
<td>82.59</td>
</tr>
<tr>
<td>Reactor Power (MWₜₜ)</td>
<td>262.0749</td>
<td>234.6</td>
</tr>
</tbody>
</table>

HTSE Layout Summary

In summary, the hydrogen production plant can be incorporated into any of several designs for a gas cooled reactor as discussed in Chapter 2. Several possibilities exist which can used to integrate the HTSE plant into a current reactor designs, but two stand out as more promising options due to their simplicity, efficiency, and design compatibility. These two designs are: 1) the extraction of turbine exhaust from the PCS to boil water, and 2) the extraction of coolant directly from the reactor via separate water boiler loops. Using an S-CO₂-GFR (Brayton Cycle), these designs were compared and contrasted on both thermodynamic and physical levels. Thermal recuperation was
maximized by recovering all the product heat via oxygen and hydrogen recuperators and feedwater preheaters. With this optimal thermal recuperation, these designs are comparable in performance, with a high thermodynamic efficiency, and each has unique physical benefits. The PCS extraction requires less in materials and capital, while the separate WB loops can perform as a self-powered decay heat safety removal system, and avoid the problem of interfering with the Brayton PCS. Upon completion of this preliminary analysis, the second design layout is recommended as the most viable layout for the integration of an HTSE hydrogen production plant.
Chapter 4 HTSE Unit

The pivotal component of nuclear hydrogen production via high temperature electrolysis is the High Temperature Steam Electrolysis (HTSE) unit. The HTSE unit utilizes an electrical current to separate water molecules into oxygen and hydrogen gas according to the following reaction:

\[ H_2O + 2e^- \rightarrow H_2 + \frac{1}{2}O_2 \]  

(4.1)

Although this unit was briefly mentioned in chapter 3 as a crucial component in the layout of a plant, no physical or theoretical description of such a unit has been undertaken up to this point. This chapter is dedicated to the physical and experimental, and theoretical discussions of the HTSE unit, as developed by Ceramatec Inc. under contract to the Idaho National Laboratory (INL).

4.1 Physical Description

There are many different designs and working models of an HTSE unit. The materials used and designs implemented are diverse. This work, however, focuses on the physical HTSE unit model developed by INL. The materials, design, and experimental implementation of a working HTSE to be discussed in the following sections, therefore, have been taken from studies completed by the INL [4.1].
The HTSE unit in this study is a stack of planar cells each stacked on a 4 inch square plate. The individual cells are stacked on this plate, and consist of 2 electrodes on either side of a solid oxide electrolyte (in this case, yttria-stabilized zirconia, or YSZ). These electrodes are porous to allow the diffusion of gas as needed. The cathode is nickel-doped zirconia cermet, while the anode is a strontium-doped lanthanum manganite. On either side of the anode is a flow channel, in which the gases flow. The channel adjacent to the anode consists of an air inflow, with an air/oxygen outflow. The channel adjacent to the cathode consists of a steam/hydrogen inflow and outflow. Both flows end up being enriched with the product gases, and their flow directions are perpendicular to one another in the horizontal plane.

The incoming stream is a mixture of steam and hydrogen gas; 90% steam by volume mixture is electrolyzed according to the reaction given by (4.1). The steam is mixed with hydrogen to ensure that the proper reducing conditions are maintained at the electrode, to prevent oxidation at the cathode. This mixture is not strictly required, however, and in this work the inclusion of hydrogen is not implemented in the calculations. In addition, 10% steam by volume is included in the outlet product stream to prevent the “drying” of the cathode. This occurs when there is not sufficient steam to completely cover the electrode, and some local deficiencies in steam inhibit the reaction, reducing efficiency. This situation will be further explained in section 4.3.3.

The electrolysis reaction (4.1) is actually composed of two half reactions, one taking place at the cathode, and one at the anode. These half reactions are:

\[ \text{H}_2\text{O} + 2\text{e}^- \rightarrow \text{H}_2 + \text{O}^= \text{(c)} \]  (4.2)
where the cathode reaction is indicated by (c) and the anode reaction is indicated by (a).

Reaction (4.2) occurs as the steam/hydrogen mixture flows past the cathode. The oxygen ions are then pulled through the ceramic oxide electrolyte, YSZ, by the electrochemical potential to undergo reaction (4.3) at the anode. The entire process is illustrated in Fig. [4.1].

Figure 4.1: Side view diagram of HTSE unit [4.1]
Each flow channel is enclosed by a separator plate, (labeled as an “interconnection” in Fig. 4.1) and then is "stacked" on top of another cell. This stack of electrolytic cells makes up the physical construct of the HTSE unit. A working experimental HTSE stack composed of 25 cells has been created, and has been used by Ceramatec/INL to obtain experimental data. A picture of this stack can be found in Fig. 4.2.

Fig. 4.2: A picture of the HTSE stack and the stack with interconnects and supports included, built and run at the INL [4.6]
4.1 HTSE Predictive Modeling

Various efforts have been made to accurately model the performance of the HTSE unit described in Chapter 4.1.1. There are 3 primary models which have been used to describe the efficiency and productivity of the HTSE unit [4.2]: 1) a simple overpotential model, as employed by Yildiz, Hohnholt, and Kazimi, 2) a 3-D model of the HTSE using FLUENT, and 3) a 1-D model using MathCAD. It is useful to explore each of these models in more detail.

4.2.1 Overpotential Model

The overpotential model was mentioned briefly in Chapter 3.2, and was employed both in this work, and in previous thermodynamic analyses completed at MIT [3.1][3.2]. In this model, the electrolysis reaction (4.1) is treated thermodynamically. It is an endothermic reaction, and the Gibbs free energy of this reaction ($\Delta G$) represents the difference in energy between the products and the reactants:

$$\Delta G_e = G_P - G_R = G_P + RT \ln \left( a_{H_2} \cdot a_{O_2}^{1/2} \right) - G_R + RT \ln \left( a_{H_2O} \right)$$  \hspace{1cm} (4.4)$$

where $\Delta G_0$ is the value of $\Delta G$ at standard conditions.

This relation can be further simplified by applying the properties of logarithms, and by noting that the activities of gases can be accurately depicted by their partial pressures. This leads us to the following equation:
\[ \Delta G_e = \Delta G_o + RT \ln \left( \frac{a_{H_2} \cdot a_{O_2}}{a_{H_2O}} \right) = \Delta G_o + RT \ln \left( \frac{P_{H_2} \cdot P_{O_2}}{P_{H_2O}} \right) \] (4.5)

where:
- \( R \) = Universal Gas Constant (J/mol*K)
- \( T \) = Temperature of the system (K)
- \( \Delta G_p \) = Gibbs free energy of the products (J/mol)
- \( \Delta G_R \) = Gibbs free energy of the reactants (J/mol)
- \( a_{H_2} \) = activity of hydrogen gas (dimensionless)
- \( a_{O_2} \) = activity of oxygen gas (dimensionless)
- \( a_{H_2O} \) = activity of steam (dimensionless)
- \( P_{H_2} \) = Pressure of hydrogen gas divided by standard pressure (dimensionless)
- \( P_{O_2} \) = Pressure of oxygen gas divided by standard pressure (dimensionless)
- \( P_{H_2O} \) = Pressure of steam divided by standard pressure (dimensionless)

Here, \( \Delta G_o \) represents the Gibbs free energy at standard temperature (298K) and a constant pressure of 1 atmosphere [4.3]. Under these conditions, we find this Gibbs energy by the following relation:

\[ \Delta G_o = -RT \ln \left( \frac{P_{H_2} \cdot P_{O_2}}{P_{H_2O}} \right) > 0. \] (4.6.a)

where the subscript \( e \) denotes equilibrium values for each species’ pressure. That is the situation when no external supply of energy is needed. Therefore:

\[ \Delta G_o = -RT \ln \left( \frac{P_{H_2} \cdot P_{O_2}}{P_{H_2O}} \right) = RT \ln \left( \frac{P_{H_2} \cdot P_{O_2}}{P_{H_2O}} \right)_e \] 4.6.b
From these relationships, one can see that the work required for electrolysis, which is directly related to the Gibbs free energy for the reaction, is directly related to the temperature of the system. As the temperature of the system increases, the Gibbs free energy for electrolysis decreases. For this reason, the HTSE operating temperatures run between 850°C and 900°C. It is at these temperatures that the Gibbs free energy for electrolysis, and thus the energy required for electrolysis of steam, becomes low enough to make the process thermodynamically attractive.

As mentioned previously, the work required for electrolysis is the Gibbs free energy. The change in Gibbs free energy represents the direct difference in electrochemical potential between the products and the reactants. A reversible process which minimizes work, therefore, would require work equivalent to the Gibbs free energy. Thus the following relationship is derived:

\[ W_{\text{min}} = -\Delta G \]  

(4.7)

where \( W_{\text{min}} \) is the minimum work required for electrolysis (kJ/mol). Because this work is required by an external source, the sign is negative, as indicated by the negative sign in front of the Gibbs free energy in (4.7). For an electrolytic cell the reversible voltage potential required for electrolysis can also be found from the Gibbs free energy by the equation:

\[ E_r = -\frac{\Delta G}{n_e F} \]  

(4.8)
where:

\[ E = \text{reversible voltage potential of the electrolytic cell} \]
\[ n_e = \text{number of electrons transferred (2 for steam)} \]
\[ \mathcal{J} = \text{Faraday number (96485 C/mol)} \]

This equation makes it possible to express the reversible cell potential in terms of the Nernst equation:

\[
E_r = -\frac{\Delta G}{n_e \mathcal{J}} = \frac{1}{n_e \mathcal{J}} (-\Delta G) = -\frac{1}{n_e \mathcal{J}} \left( \Delta G_o + RT \ln \left( \frac{P_{H_2e} * P_{O_{2e}}^{\frac{1}{2}}}{P_{H_2O_e}} \right) \right)
\]

\[
E_r = E_o - \frac{1}{n_e \mathcal{J}} RT \ln \left( \frac{P_{H_2e} * P_{O_{2e}}^{\frac{1}{2}}}{P_{H_2O_e}} \right).
\] (4.9)

Although the reversible cell potential represents the difference in energy between the reactants and products of an electrolytic cell, this value is not a realistic representation of the actual potential required for electrolysis. To expect the needed energy to be only the reversible work in an electrolytic cell is not practical due to energy losses that come from certain irreversibilities of the electrolysis system. There are three primary categories of realistic energy losses which prevent the achievement of reversible electrolysis: 1) activation losses 2) mass transfer losses and 3) ohmic resistance losses.

Activation losses, denoted by ‘\(a\)’, relate to the energy required to “activate” the electrolysis system evolving hydrogen and oxygen at the electrodes. Mass transfer losses, denoted by ‘\(c\)’ representing the energy required for each species to move to and from the electrode as well as within the porous matrix of the electrodes. Ohmic resistance losses, denoted by ‘\(\Omega\)’ relate to the energy required to move the ions across the potential gradient.
Because of each of these losses, an additional amount of work must be input into the system. This additional work represents an increased amount of potential that must be applied to the cell in order for it to operate at steady state. The difference between the reversible cell potential, and the actual operating cell potential is known as the overpotential ($\eta$). The overpotential is the overall potential required to overcome each of the 3 mechanisms of irreversible energy loss, and thus can be considered the sum of three smaller overpotentials ($\eta_a + \eta_c + \eta_\alpha$). Thus, the operating potential can be determined by:

$$E = E_o - \frac{1}{nF}RT \ln\left(\frac{P_{H_2} \cdot P_{O_2}^{1/2}}{P_{H_2O}}\right) - (\eta_a + \eta_c + \eta_\alpha) \quad (4.10)$$

As the current density (A/cm$^2$) of the electrodes changes, the values of each of these overpotentials change according to different mechanisms. At different values of current density, a different mechanism may be the major cause of potential loss. This can be demonstrated by Fig. [4.3].
Figure 4.3: Dependence of SOEC cell voltage and power density on current density (Example plot for theoretical modeling of an LSM-YSZ-Ni/YSZ system at 700 °C) [3.2]

The current density is directly rated to the hydrogen production rate within the cell, therefore assuming a small current density simply to reduce the overpotential is not acceptable. Accordingly, the objective in selecting appropriate HTSE unit models is to determine which setup, materials, and process conditions lead to a minimal overpotential while maximizing the current density and thus hydrogen production rate. A model which can accomplish these things can minimize irreversibilities, and thus provide a more precise analysis of the process than the approach employed in this work.

Finally, for comparative purposes, the efficiency of an electrolytic cell such as the HTSE unit is given by the following relationship:

$$\eta = \frac{E_r}{E}$$  \hspace{1cm} (4.11)
In the thermodynamic analyses presented in Chapter 3.2, an overpotential value of 10% was utilized. This gave a HTSE efficiency of 91%, and this value was used to characterize the HTSE unit in our work. This is simply an estimated value, however. Future work should be done to develop a model to determine the hydrogen production rate, as well as the optimal setup and operating conditions for the HTSE for inclusion in the calculations described in Chapter 3.

4.2.2 3-D Model [3.5]

A 3 dimensional model of an individual HTSE unit cell has been completed by the INL. In this model, the computational fluid dynamics (CFD) software FLUENT was

Figure 4.4: FLUENT electrolysis stack model depiction of the HTSE single cell in 3 forms: to scale, 10x enlargement, and an exploded view of the cell [3.5]
used to create a fully 3-D flow model of an HTSE cell coupled to a high-temperature helium cooled reactor. A detailed description of this model can be found in [4.5] while a simplified description will be repeated here.

The model consists of the layers depicted in Fig. 4.4: two separator plates, with edge rails on either side of the flow channel to guide the fluid flow, the electrodes, and finally the electrolyte surrounded by an insulator. As seen in the diagram, the flow channels are perpendicular to each other in the horizontal plane. The vertical boundaries of the fluent model consist of two planar symmetry boundaries, one located half way through each separator plate. The flow channels for gas flow were both defined in FLUENT as high-porosity porous media regions with metallic nickel as the solid material for the steam/hydrogen channel, and ferritic stainless steel for the oxygen/air channel. These channels are modeled to have anisotropic permeability, high in the direction of gas flow, but low in opposing and perpendicular directions. The height of these flow channels was set at 1.019 mm. For the middle 3 layers (electrodes and electrolyte) a FLUENT solid-oxide fuel cell (SOFC) module was used. This module treats the solid oxide electrolyte layer as a 2-D planar element with similar properties to YSZ, but it treats the electrodes as fully 3-D volumes. Thus the thickness of these three layers is modeled as the thickness of the 2 electrodes only (0.1 mm), while in reality this thickness would also include the thickness of the electrolyte (0.2 mm). The electrolyte in the FLUENT model is also surrounded with a 2-D “insulator” layer which prevents ionic transfer, and has the properties of YSZ. This was done to prevent shorts between the side rails and the electrodes. In addition to these parameters, the current density and several
gap electrical contact resistances were input into the model based upon empirical data obtained from HTSE stack performance data. Finally, flow inlets, compositions, and the modified SOFC subroutine were input into FLUENT, and the results will be discussed in section 4.2.4.

A major accomplishment of this model was to predict and help understand the “dryout” [4.6] phenomenon mentioned previously. If the steam content of the product hydrogen stream is too small, regions of steam deficits appear, which hinder the electrolysis reaction. The formation of these regions is known as dryout, and they have been observed generally on the region indicated in Fig. 4.5. This is the region that suffers dryout most due to the reduced oxygen and steam content. This reduced steam and oxygen slows the overall reaction, which ultimately prevents further electrolysis in this region from occurring.
Figure 4.5: Depiction of region where dryout occurs on the surface of a cathode in the electrolysis stack unit as predicted by FLUENT 3-D model

4.2.3 1-D model [3.5]

The 1-D HTSE model created by INL determines the voltage required to run the electrolysis stack, as well as the temperature change associated with the electrolysis reaction. The inputs for this model are the current densities, the enthalpies of each material as a function of temperature, the heat transfer in the system (for each case discussed below, the system is considered adiabatic), and the stack area specific resistance. Other inputs include the known flow rates of the reactants and products as
well as the initial temperature of the reactants. The model consists of an iterative
calculation of the product temperature ($T_p$), the Operating Voltage ($V_{op}$), and the
electrical work required ($\dot{W}$) to run the cell. The work is found according to the
following statement of the 1st law of thermodynamics for a control volume with streams
of fluids:

$$\dot{Q} - \dot{W} = \sum \dot{N}_i \left[ \Delta H_i^* + H_i(T_p) - H_i^* \right] - \sum \dot{N}_i \left[ \Delta H_i^* + H_i(T_R) - H_i^* \right]$$ (4.12)

where:
- $\dot{Q}$ = Heat transfer to or from the system
- $\dot{N}_i$ = Molar flow rate of the $i^{th}$ product or reactant
- $\Delta H_i^*$ = Heat of formation of the $i^{th}$ product or reactant
- $H_i(T_p) - H_i^*$ = Sensible heat for the $i^{th}$ product or reactant

The product temperature must first be guessed, and then the values based upon
that temperature used in (4.12). The hydrogen production rate, as well the minimum
steam feed rate, are both set for a particular current density, and can be found according
to the following relation:

$$\dot{N}_{i,H_2O,min} = \Delta \dot{N}_{H_2O} = \frac{I}{23} N_{cells} = \frac{i A_{cell}}{23} N_{cells} = \Delta \dot{N}_{H_2}$$ (4.13)

where:
- $\dot{N}_{i,H_2O,min}$ = Minimum steam flow required for electrolysis (mol/sec)
- $N_{cells}$ = Number of cells in the stack
- $\Delta \dot{N}_{H_2}$ = Rate of Hydrogen Production(mol/sec)
- $I$ = current
- $i$ = current density
$A_{\text{cell}}$ = Active area of the electrolytic cell

With this in mind, the relation for the average Nernst potential throughout the cell is given by:

$$
\bar{V} = \frac{1}{2RT_P(T - T_R)\left(y_{o,0_2,A} - y_{i,0_2,A}\right)\left(y_{o,H_2,C} - y_{i,H_2,C}\right)} \int \int \int \Delta G_f(T) + RT \ln \left(\frac{1 - y_{H_2}}{y_{H_2} y_{o_2}^2} \right) dy_{H_2} dy_{o_2} dT
$$

(4.14)

where:

$y_{o,0_2,A} - y_{i,0_2,A}$ = change in mole fraction of oxygen across the anode

$y_{o,H_2,C} - y_{i,H_2,C}$ = change in mole fraction of hydrogen across the anode

$1 - y_{H_2}$ = mole fraction of steam

$y_{H_2}$ = mole fraction of hydrogen

$y_{o_2}$ = mole fraction of oxygen

Again, this requires that the final temperature of the product gases be guessed until the actual temperature can be determined by iteration. Once the average Nernst potential throughout the cell is obtained, the following relation can be used to determine the operating cell potential at the given product temperature:

$$
V_{op} = \bar{V} + i A SR(T)
$$

(4.15)

where the stack area-specific resistance as a function of temperature is represented by $ASR(T)$. Once these equations have been used based upon the guessed value of the product temperature, a fully iterative process can be used to determine the actual product.
gas temperature. The INL has used MathCAD [4.7] to perform this iteration, and the algorithm used for this work is found in Appendix A. For further discussion of the implications and mathematical background of this model, one can refer to [3.5] for the complete presentation of the 1-D HTSE electrolysis stack model.

4.2.4 Model Results

Both the 3-D FLUENT model and the 1-D MathCAD model yielded process data that can be entered into ASPEN or HYSYS (a chemical engineering plant design program similar in design and scope to ASPEN [4.8]) to provide an accurate depiction of the HTSE unit in a process model.

![Comparison of a) stack operating cell voltage versus current density for the FLUENT model along with several experimental values, and b) HTSE outlet temperatures versus stack operating voltage for the FLUENT model along with several experimental values [3.5]](image_url)

Figure 4.6
The FLUENT model can be used to determine local and specific conditions within the cell. The prediction and causation of a dryout region is derived by this model. The overall conditions such as the average Nernst potential, the cell operating potential, the stream temperatures, and the heat of reaction are also predicted. The operating cell potential of the 3-D model was graphed against several experimental values to determine the validity of the model. The experimental values were obtained from four small inconel-sheathed thermocouples that were inserted into selected flow channels of the operating stack at INL [4.9]. The results seen are a result of a DC sweep of the stack while the thermocouples recorded the data. The results of the comparison between the FLUENT model and these experimental results can be seen in Fig. 4.6. As can be seen in the graph on the left, very good agreement exists between the FLUENT model and the experimental results of the stack process runs. A comparison of the FLUENT model temperature predictions based on the stack operating voltage can also be seen in the graph on the right. The temperatures do not exactly match between the model and the experimental runs, partly because the DC sweep was so swift that temperatures were not allowed to reach steady state. However, while the FLUENT models temperatures do not precisely match the experimental temperatures, the similar trends of both temperatures are clearly seen, indicating an accurate model [3.5].

While the FLUENT model itself accurately depicts the conditions within the cell, the 3-D model is far too complex to utilize in the plant layout software. The 1-D model is simple enough that it can be adapted and input in such software as a user defined subroutine. With this in mind, a comparison was made between the 1-D and 3-D models to determine whether the 1-D MathCAD model could match the accuracy of the 3-D
FLUENT model. The results of this comparison can be seen in Fig. 4.7. The operating voltage predicted by the 1-D model is slightly higher than the value predicted by the FLUENT model. Since a higher voltage indicates a lower efficiency, the 1-D model is actually more conservative, and thus appropriate for use in layout modeling. This

![Graph showing predicted operating voltage and gas outlet temperatures](image)

**Figure 4.7:** Predicted operating voltage and gas outlet temperatures for adiabatic HTSE stack operation; comparison of 1-D integral MathCAD model with full 3-D FLUENT simulation [3.5]

difference is due to the 1-D model’s inability to account for local changes and non-idealities in the electrolytic cell, which can be predicted by the FLUENT model.

Because the 1-D model matches well with the 3-D model and experiments, it is acceptable to use as a basis for modeling plant layouts using ASPEN. Though the present work focused only on utilizing the overpotential model, the INL plant layouts, which are used as a benchmark for this work, utilized a user defined model in HYSYS to represent the HTSE unit based upon the 1-D model discussed here.
4.3 HTSE Unit Summary

A multi-cell working HTSE experimental unit has been created by Ceramatec/INL. Each electrolytic cell consists of a microfilm anode, cathode, and electrolyte layer, all held between two flow channels. Several of these cells are stacked on top of each other to form the HTSE unit. The flow channels allow both the inlet streams to contact the electrodes, facilitating the reaction described by equation 4.1. A working experimental sized HTSE has been built, tested, and used to gather data at the INL. In addition, 3 models have been used to model the functions of the HTSE unit. The first is an overpotential model, which predicts the overall potential needed for the cell based upon irreversible voltage drops within the HTSE unit. The second is a fully 3-D FLUENT model which depicts the entire HTSE cell and determines local conditions as well as the mean values of global parameters. Finally, a 1-D MathCAD model has been developed (which gives a more conservative estimate than the others) which can be used to determine overall process conditions within the HTSE stack.

The present work utilizes the overpotential model to determine the operating conditions and energy requirements of the HTSE unit. From this, an optimal integration of the HTSE unit with the GFR is developed, as described in Chapter 3. The INL models of the HTSE plant layout, however, utilize the 1-D model to determine the process conditions and energy requirements of the HTSE unit. Therefore, the layout used by the INL for the HTSE plant is slightly different than the one included in this work. This INL layout is described in Chapter 5, and is similar enough to the overpotential-model-generated layout that it is used as a benchmark to compare with our results.
Chapter 5 Modeling, Results, and Benchmarking

The modeling efforts involved in this thesis were performed using several different software platforms and computational codes. In this chapter, the methods for modeling the various integrated layouts for a hydrogen production plant are described in more detail. Many designs had been investigated; however, the methods used to model these designs fell into two primary categories, as described below. In addition to this description, the INL plant layout and the modeling techniques employed by the INL for their integrated HTSE/GFR plant are presented. Finally, the results of the optimally integrated layout selected in this Thesis and the results of the INL integrated layout are documented, and the calculations described in this thesis benchmarked against the results obtained by the INL.

5.1 MIT Modeling and Results

Two different methods were used to determine the numerical results of the previously described models. For the plant layout depicted in Figure 3.3 and related layouts, a thermodynamic plant design code previously created by Dostal [2.9] was used to determine the properties of the S-CO₂-GFR PCS. This code was based upon a direct recompression cycle for the S-CO₂-GFR system described in section 1.4, and required several different descriptive parameters. Required inputs to operate this code include: the pressure drops for the cycle, the turbomachinery isentropic efficiencies, the fraction of flow to the precooler, the pressure ratio for the cycle, the main compressor outlet
Table 5.1: Input parameters for thermodynamic code created for two options:
Direct CO₂ extraction from the reactor (method 1) and extraction from
the turbine exhaust (method 2)

<table>
<thead>
<tr>
<th></th>
<th>Method 1</th>
<th>Method 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fractional Pressure Drops</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IHX-Reactor</td>
<td>2.50%</td>
<td>2.50%</td>
</tr>
<tr>
<td>Intercooler</td>
<td>0.13%</td>
<td>0.13%</td>
</tr>
<tr>
<td>Hot recuperator, hot steam</td>
<td>2.14%</td>
<td>2.14%</td>
</tr>
<tr>
<td>Hot recuperator, cold steam</td>
<td>0.29%</td>
<td>0.29%</td>
</tr>
<tr>
<td>Cold recuperator, hot steam</td>
<td>0.24%</td>
<td>0.24%</td>
</tr>
<tr>
<td>Cold recuperator, cold steam</td>
<td>0.09%</td>
<td>0.09%</td>
</tr>
<tr>
<td>Water-Steam/CO₂ exchanger</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Turbine Efficiency</td>
<td>90%</td>
<td>90%</td>
</tr>
<tr>
<td>Compressor Efficiency (both)</td>
<td>89%</td>
<td>89%</td>
</tr>
<tr>
<td>HT Recuperator Effectiveness</td>
<td>96%</td>
<td>96%</td>
</tr>
<tr>
<td>LT Recuperator Effectiveness</td>
<td>84.4%</td>
<td>84.4%</td>
</tr>
<tr>
<td>Fractional Flow Through Pre-cooler</td>
<td>60%</td>
<td>60%</td>
</tr>
<tr>
<td>Pressure Ratio</td>
<td>2.63</td>
<td>2.63</td>
</tr>
<tr>
<td>Main Compressor Outlet Pressure (MPa)</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td>Reactor Outlet Temperature (°C)</td>
<td>650</td>
<td>650</td>
</tr>
<tr>
<td>Fraction of Turbine Exhaust to IHX</td>
<td>0%</td>
<td>9.20%</td>
</tr>
</tbody>
</table>

pressure, the main compressor inlet temperature, and the reactor outlet temperature. The values used for each of these inputs are listed in Table 5.1. A key to interpret Table 5.1 and the flowsheets is included in Table 5.2. The code provides the work of the compressors, the work of the turbine, and the PCS thermodynamic efficiency as output.
The values provided by this code were then used in coordination with the ASPEN model to determine the overall hydrogen production efficiency, as described below.

<table>
<thead>
<tr>
<th>Label</th>
<th>Component</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>WB</td>
<td>Water Boiler</td>
<td>Process steam for HTSE circuit</td>
</tr>
<tr>
<td>IHX</td>
<td>Intermediate Heat Exchanger</td>
<td>Water boiler; different name for same unit</td>
</tr>
<tr>
<td>HT Recuperator</td>
<td>High Temperature Recuperator</td>
<td>Recovering high temperature heat in Brayton recompression cycle</td>
</tr>
<tr>
<td>LT Recuperator</td>
<td>Low Temperature Recuperator</td>
<td>Recovering low temperature heat in Brayton recompression cycle</td>
</tr>
<tr>
<td>B1</td>
<td>Steam Turbine</td>
<td>Generate power used to circulate HTSE circuit</td>
</tr>
<tr>
<td>B3</td>
<td>Flow Splitter</td>
<td>Separate steam into two streams</td>
</tr>
<tr>
<td>O2RECUP</td>
<td>Oxygen Recuperator</td>
<td>Heat steam using oxygen product</td>
</tr>
<tr>
<td>H2RECUP</td>
<td>Hydrogen Recuperator</td>
<td>Heat steam using hydrogen product</td>
</tr>
<tr>
<td>B6</td>
<td>Flow Joiner</td>
<td>Merge two steam flows into single HTSE feed stream</td>
</tr>
<tr>
<td>OH</td>
<td>Ohmic Heater</td>
<td>Provide extra heat to steam</td>
</tr>
<tr>
<td>HTSE</td>
<td>High Temperature Steam</td>
<td>Electrolyze Steam into Hydrogen and Oxygen</td>
</tr>
<tr>
<td>Electrolysis Unit</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B8</td>
<td>Separator</td>
<td>Used by ASPEN to separate products (not physically present)</td>
</tr>
<tr>
<td>B11</td>
<td>Flow Joiner</td>
<td>Used for simplicity in ASPEN; streams are not actually merged</td>
</tr>
<tr>
<td>B12</td>
<td>Pre-Heater</td>
<td>Heat feedwater prior to WB</td>
</tr>
</tbody>
</table>

The second method was used to determine the numerical results for the layout depicted in Fig. 3.4 as well as certain related layouts. This method was completely identical to the method indicated previously, only that an additional input was defined: the fraction of the turbine exhaust that was used to boil the water in the IHX was
included, as this influenced the performance of the PCS. Once the output for this adaptation of the code was obtained, the values were used in coordination with ASPEN as in the previous method.

The ASPEN model was based upon the HTSE plant designs described in chapter 3. The layouts of these plants are depicted in Fig. 5.1 and Fig. 5.2. Although these layouts show the reactor as the heat source, the heat source for the extraction from the PCS turbine exhaust layout depicted in Fig. 5.2 was programmed in the model by simply adapting the "reactor" properties to match those of the turbine exhaust.

![Image: Schematic of ASPEN model integrated plant layout for direct-from-reactor extraction (corresponding to Fig. 3.4)](image_url)

**Figure 5.1:** Schematic of ASPEN model integrated plant layout for direct-from-reactor extraction (corresponding to Fig. 3.4)
To evaluate the overall efficiency of the hydrogen production plant, and to determine energy requirements and thermal recuperation possibilities, the HTSE portion was modeled using ASPEN. Each of the components of the HTSE plant was programmed into ASPEN using certain deterministic models and properties.

For the HTSE unit itself, the overpotential model described in section 4.2.1 was incorporated into ASPEN as the deterministic model, while the operating conditions were defined as 900°C and 6 MPa. The reactor was programmed in ASPEN differently.
depending on which integration method was being investigated. To determine the HTSE performance in the turbine exhaust extraction integration scheme, the heat source was modeled as a furnace providing a constant heat input to the IHX, corresponding to the overall CO₂ draw of 9.2% from the turbine exhaust. For the integration scheme involving heat extraction directly from the reactor, the reactor itself was modeled as a furnace with appropriate outlet temperatures and pressures, and a heat generation rate corresponding to 9.2% of that generated by the reactor. The coolant flow was scaled down to model an appropriate amount of heat (9.2%) being extracted from the reactor.

The compressor of the HTSE plant was programmed as a basic isentropic compressor with an efficiency of 89%, and the turbine was similarly programmed as a basic isentropic device with an efficiency of 90%. Each of the heat exchangers utilized a minimum approach temperature method having a value of 30°C. This temperature represents the minimum temperature difference allowed between the cold and hot streams. The separator shown in the layouts was approximated as a preliminary separator with 100% efficiency in separating the streams. In reality, the oxygen and hydrogen streams never mix, so there is no need for a separator; this unit is simply a dummy unit used for convenience in ASPEN.

<table>
<thead>
<tr>
<th>Feed Streams</th>
<th>Temp. (°C)</th>
<th>Pressure (Mpa)</th>
<th>Flow Rate(kg/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S-CO₂ From Reactor</td>
<td>650</td>
<td>20</td>
<td>1143.152</td>
</tr>
<tr>
<td>Feed Water</td>
<td>30</td>
<td>0.1</td>
<td>93</td>
</tr>
<tr>
<td>Flow Fraction to Hydrogen</td>
<td>-</td>
<td>-</td>
<td>59.19</td>
</tr>
<tr>
<td>Recuperator</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>
In addition to these input parameters, feed stream properties are input into the reactor, as shown in Table 5.3. Any streams not listed in this table are left to be determined by ASPEN.

The ASPEN model uses this input information to perform the mass and energy balances described in section 3.3. The output of the ASPEN model is a list of the complete thermodynamic properties of each stream including temperature, flow rate, pressure, and chemical composition. For a complete listing of the calculations and iterations completed by ASPEN, refer to Appendix B.

Once the thermodynamic properties of all the HTSE streams were determined, the output from the code developed by Dostal was used in combination with this data to determine the overall properties of an integrated plant. These calculations were performed using MathCAD, and the complete set of calculations is provided in Appendix B. Of special import among the calculated integrated plant properties are the PCS efficiencies for each integration method, and the overall hydrogen production efficiencies for each integrated plant, as these are used as one of the primary methods of comparison, as described in chapter 3. A complete list of the overall integrated plant properties for the optimal integration scheme (shown in Fig. 5.1) can be found in Table 5.4.
Table 5.4: Properties of all streams in the separate WB loops integrated plant

<table>
<thead>
<tr>
<th>Stream ID</th>
<th>1</th>
<th>2</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>C</td>
<td>349.4</td>
<td>196.4</td>
<td>196.4</td>
<td>870.0</td>
<td>196.4</td>
<td>870.0</td>
</tr>
<tr>
<td>Pressure</td>
<td>bar</td>
<td>163.000</td>
<td>60.000</td>
<td>60.000</td>
<td>60.000</td>
<td>60.000</td>
<td>60.000</td>
</tr>
<tr>
<td>Vapor Frac</td>
<td>km/d/hr</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
</tr>
<tr>
<td>Mole Flow</td>
<td>kg/hr</td>
<td>18584.244</td>
<td>18584.224</td>
<td>6788.817</td>
<td>6788.817</td>
<td>11795.407</td>
<td>11795.407</td>
</tr>
<tr>
<td>Mass Flow</td>
<td>kg/hr</td>
<td>334799.997</td>
<td>334799.997</td>
<td>122302.439</td>
<td>122302.439</td>
<td>212497.6</td>
<td>212497.558</td>
</tr>
<tr>
<td>Volume Flow</td>
<td>cum/hr</td>
<td>3438.923</td>
<td>7143.951</td>
<td>2609.684</td>
<td>10738.739</td>
<td>4534.264</td>
<td>18658.302</td>
</tr>
<tr>
<td>Mass Flow</td>
<td>kg/hr</td>
<td>334799.997</td>
<td>334799.997</td>
<td>122302.439</td>
<td>122302.439</td>
<td>212497.558</td>
<td>212497.558</td>
</tr>
<tr>
<td>CARBO-01</td>
<td>WATER</td>
<td>334799.997</td>
<td>334799.997</td>
<td>122302.439</td>
<td>122302.439</td>
<td>212497.558</td>
<td>212497.558</td>
</tr>
<tr>
<td>HYDRO-01</td>
<td>WATER</td>
<td>334799.997</td>
<td>334799.997</td>
<td>122302.439</td>
<td>122302.439</td>
<td>212497.558</td>
<td>212497.558</td>
</tr>
<tr>
<td>OXYGE-01</td>
<td>WATER</td>
<td>334799.997</td>
<td>334799.997</td>
<td>122302.439</td>
<td>122302.439</td>
<td>212497.558</td>
<td>212497.558</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stream ID</th>
<th>10</th>
<th>11</th>
<th>13</th>
<th>14</th>
<th>15</th>
<th>16</th>
<th>17</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>C</td>
<td>900.0</td>
<td>900.0</td>
<td>900.0</td>
<td>248.2</td>
<td>900.0</td>
<td>130.0</td>
</tr>
<tr>
<td>Pressure</td>
<td>bar</td>
<td>60.000</td>
<td>60.000</td>
<td>60.000</td>
<td>60.000</td>
<td>60.000</td>
<td>60.000</td>
</tr>
<tr>
<td>Vapor Frac</td>
<td>km/d/hr</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
</tr>
<tr>
<td>Mole Flow</td>
<td>kg/hr</td>
<td>27876.336</td>
<td>9292.112</td>
<td>18584.224</td>
<td>27876.336</td>
<td>18584.224</td>
<td>27876.336</td>
</tr>
<tr>
<td>Mass Flow</td>
<td>kg/hr</td>
<td>334799.997</td>
<td>297336.432</td>
<td>37463.656</td>
<td>37463.656</td>
<td>334799.997</td>
<td>334799.997</td>
</tr>
<tr>
<td>Volume Flow</td>
<td>cum/hr</td>
<td>45860.278</td>
<td>15310.016</td>
<td>30549.900</td>
<td>20634.119</td>
<td>30206.482</td>
<td>16008.669</td>
</tr>
<tr>
<td>Enthalpy</td>
<td>MMkc/ al/hr</td>
<td>179.926</td>
<td>64.196</td>
<td>115.726</td>
<td>44.318</td>
<td>-927.430</td>
<td>20.607</td>
</tr>
<tr>
<td>Mass Flow</td>
<td>kg/hr</td>
<td>334799.997</td>
<td>334799.997</td>
<td>122302.439</td>
<td>122302.439</td>
<td>212497.558</td>
<td>212497.558</td>
</tr>
<tr>
<td>CARBO-01</td>
<td>WATER</td>
<td>334799.997</td>
<td>334799.997</td>
<td>122302.439</td>
<td>122302.439</td>
<td>212497.558</td>
<td>212497.558</td>
</tr>
<tr>
<td>OXYGE-01</td>
<td>WATER</td>
<td>297336.432</td>
<td>297336.432</td>
<td>297336.432</td>
<td>297336.432</td>
<td>297336.432</td>
<td>297336.432</td>
</tr>
<tr>
<td>Stream ID</td>
<td>FEEDH20</td>
<td>H2</td>
<td>O2</td>
<td>RIN</td>
<td>ROUT</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temperature</td>
<td>C</td>
<td>81.5</td>
<td>250.8</td>
<td>245.4</td>
<td>486.3</td>
<td>650.30</td>
<td></td>
</tr>
<tr>
<td>Pressure</td>
<td>bar</td>
<td>2.000</td>
<td>60.000</td>
<td>60.000</td>
<td>200.000</td>
<td>200.000</td>
<td></td>
</tr>
<tr>
<td>Vapor Frac</td>
<td>km/d/hr</td>
<td>0.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td></td>
</tr>
<tr>
<td>Mole Flow</td>
<td>kg/hr</td>
<td>18584.224</td>
<td>18584.224</td>
<td>9292.112</td>
<td>93509.790</td>
<td>93509.790</td>
<td></td>
</tr>
<tr>
<td>Mass Flow</td>
<td>kg/hr</td>
<td>334799.997</td>
<td>37463.565</td>
<td>297336.432</td>
<td>31372.635</td>
<td>38262.178</td>
<td></td>
</tr>
<tr>
<td>Volume Flow</td>
<td>cum/hr</td>
<td>463.470</td>
<td>13822959</td>
<td>6819.490</td>
<td>31372.635</td>
<td>38262.178</td>
<td></td>
</tr>
<tr>
<td>Mass Flow</td>
<td>kg/hr</td>
<td>334799.997</td>
<td>37463.565</td>
<td>297336.432</td>
<td>31372.635</td>
<td>38262.178</td>
<td></td>
</tr>
<tr>
<td>CARBO-01</td>
<td>WATER</td>
<td>334799.997</td>
<td>334799.997</td>
<td>122302.439</td>
<td>122302.439</td>
<td>212497.558</td>
<td>212497.558</td>
</tr>
<tr>
<td>OXYGE-01</td>
<td>WATER</td>
<td>297336.432</td>
<td>297336.432</td>
<td>297336.432</td>
<td>297336.432</td>
<td>297336.432</td>
<td>297336.432</td>
</tr>
</tbody>
</table>
5.2 Idaho National Lab Modeling and Results [3.8]

The Idaho National Laboratory performed preliminary plant integration calculations for a 600 MW\text{th} plant similar to the calculations presented in this thesis. The chemical engineering plant design software used was HYSYS [4.8], which is very similar to ASPEN, and was in fact developed by the same company. Some differences are found in the plant layout investigated by the INL.

The first primary difference is that the full scale 1-D model was employed in HYSYS rather than the overpotential-estimated model used by the author of this thesis. This 1-D model, as described in section 4.2.3, is more comprehensive than the overpotential model, and therefore more accurately models the working conditions of the HTSE unit.

The second primary difference is an adaptation to the layout of the HTSE plant itself. As indicated in section 4.2.2, dryout is a problem that occurs when insufficient steam is available for electrolysis in the HTSE cells. To alleviate this problem, a portion of hydrogen is included in the feed stream to the HTSE unit equivalent to 10% by volume. Additionally, the fractional conversion is adjusted so that the product stream contains 10% steam along with the hydrogen. By adjusting the feed and product streams of the HTSE in this way, dryout is prevented. The layout used by the INL is adapted to provide these flow compositions. This adapted layout is shown in Fig. 5.3.
Figure 5.3: INL’s HYSYS model plant layout as designed for 600 MWth plant [3.8]

With the exception of these two differences, similar procedures were used to determine the resulting efficiency and integrated plant properties. These results included data for the HTSE unit as well as the overall plant properties, as the 1-D model facilitated calculation of these properties as well. The results of the INL’s integrated plant calculations are summarized in Table 5.5.

<table>
<thead>
<tr>
<th>Table 5.5: Results of INL’s full scale GFR-HTSE plant calculations</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Reactor Power</strong></td>
</tr>
<tr>
<td><strong>H₂ Production</strong></td>
</tr>
<tr>
<td>Overall process efficiency</td>
</tr>
<tr>
<td>Rate based on LHV</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Water Consumption</strong></td>
</tr>
<tr>
<td><strong>Electrolysis Cell Operating Conditions</strong></td>
</tr>
<tr>
<td>Temperature</td>
</tr>
<tr>
<td>Pressure</td>
</tr>
<tr>
<td>Inlet mole fractions, H₂O/H₂</td>
</tr>
<tr>
<td>Outlet mole fraction, H₂O/H₂</td>
</tr>
<tr>
<td>Volumetric H₂+H₂O flow rate</td>
</tr>
<tr>
<td>Volumetric O₂ flow rate (generated)</td>
</tr>
<tr>
<td>Current Density</td>
</tr>
<tr>
<td>Cell Operating Voltage</td>
</tr>
</tbody>
</table>
5.3 Benchmarking

Though slightly different methods and layouts were used by the INL and this work, the basic principles were similar. To benchmark the work accomplished by this thesis, a comparison of the results will now be undertaken. The data shown in Table 5.5 is for a 600 MWth plant, with the overall plant layout shown in Fig. 5.3 but a direct scale-up factor of four can provide suitable data for comparison. During steady state operations, the differences between Fig. 5.3 and Fig. 5.1 do not greatly change the mass and energy balances. Additionally, if the overpotential value used (10%) is equivalent to the overall losses of the 1-D model at 800°C used by the INL, the hydrogen production rate and overall hydrogen efficiencies can be compared to provide an acceptable benchmark.

Table 5.6 provides a comparison of the two layout models, as indicated by the results discussed in the previous chapter. As can be seen, the hydrogen production rate, and the overall hydrogen efficiencies for the layout designs developed by both the INL and MIT (10% overpotential) are very similar, differing by only 3.94% and -5.71%, respectively. For the sake of an upper limit analysis, the 0% overpotential model is also included in the comparison, indicating the upper limit for which the INL model could be benchmarked with the MIT model. Though each of these models is slightly different, this small difference between the overall hydrogen efficiency and the hydrogen production rate confirms the validity of the methods and computations employed in the present work.
Table 5.6: Comparison of results for INL 1-D model and MIT 10% and 0% Overpotential Models

<table>
<thead>
<tr>
<th></th>
<th>INL 1-D</th>
<th>MIT 10% Overpotential</th>
<th>MIT 0% Overpotential</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen Production Efficiency</td>
<td>50%</td>
<td>47.30%</td>
<td>-5.71%</td>
</tr>
<tr>
<td>Overall Hydrogen Production Rate (kg/s)</td>
<td>10</td>
<td>10.41</td>
<td>3.94%</td>
</tr>
</tbody>
</table>

5.4 Sensitivity Analysis

The numbers provided for this thesis are for the simple cases in which temperatures range from 550°C to 750°C, while the balance of process variables were held constant. It is also worthwhile to determine what influence other process variables may have on the hydrogen production using GFR-HTSE. To determine which process variables have a significant influence on hydrogen production efficiencies and rates, a sensitivity analysis was performed based upon perturbations in the following properties while holding the reactor outlet temperature constant at 650°C:

1. Temperature of products
2. Efficiency of product heat exchangers
3. Feedwater temperature and pressure
4. Overpotential of HTSE
5. Amount of heat (coolant) withdrawn from the PCS

The results of this analysis provide insight as to which process variables have the strongest influence on the hydrogen production process. The sensitivity of the temperature and pressure of the HTSE unit, though significant to the hydrogen production rate and the hydrogen production efficiency, have been analyzed previously.
by the INL [3.5][3.8][4.1]. These studies culminated in the identification of the operating voltage described in chapter 4.2.3.

5.4.1. Temperature of HTSE Products

Each of the HTSE ASPEN simulations was performed assuming that the preheater, which utilized the low quality product heat to raise the feedwater temperature, had a standard hot-side temperature limit. This limit was held constant at around 130°C for each of the simulations. In this sensitivity analysis, the temperature limit was adjusted to higher and lower values, and the hydrogen production rates and efficiencies were reevaluated. These results can be found in Table 5.7.

Table 5.7: Influence of Product Temperature on Hydrogen Production Rate and Overall Hydrogen Production Efficiency

<table>
<thead>
<tr>
<th>Preheater hot-side outlet temp</th>
<th>H2 Flow Rate (kg/s)</th>
<th>Fractional Change (%)</th>
<th>Efficiency (%)</th>
<th>Fractional Change (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>130°C</td>
<td>10.41</td>
<td>-</td>
<td>47.3</td>
<td>0</td>
</tr>
<tr>
<td>30°C</td>
<td>11.56</td>
<td>11.05</td>
<td>47.3</td>
<td>0</td>
</tr>
<tr>
<td>160°C</td>
<td>10.02</td>
<td>-3.75</td>
<td>47.3</td>
<td>0</td>
</tr>
</tbody>
</table>

Because the preheater heats the feedwater prior to heat from the reactor boiling the water, if the reactor draw is held constant, no efficiency gain is attained, as seen in Table 5.7. This is because the overall heat inputs remain constant. The effect of adjusting this limit, however, is to allow for a variance in flow rate of water. The upper limit of this flow rate, as found in this analysis, depends upon the outlet conditions of the
water boiler; if the feedwater flow rate is too high, the vaporization heat requirement for the feedwater is not met by the water boiler, and an exit quality of less than 1 results. This can cause severe corrosion problems in the steam turbine, and therefore must be avoided. This boundary leads to the hydrogen production rates evaluated in Table 5.7.

Nearly identical to the product outlet temperatures, the temperature and pressure of the feedwater affect the amount of steam that can be electrolyzed. A higher feedwater temperature (pressure) correlates to a higher allowable water flow rate, and thus a higher hydrogen production rate. Again, this higher flow rate is limited by the heat draw from the reactor; if the reactor heat draw is too small to sufficiently superheat the steam, liquid condensate will form in the steam turbine, causing unacceptable corrosion problems.

5.4.2. Efficiency of Product Heat Exchangers

In the analyses described in section 3, the product recuperators were modeled by assuming a minimum approach temperature. This limit was held at 30°C throughout the modeling process. In this sensitivity analysis, this valued was decreased while all other variables were held constant in order to determine its overall influence on the hydrogen production rates and efficiencies. Because there is no additional heat input or recuperation, no production rate fluctuations are produced in throughout these perturbations. The increase of heat from the product recuperators does decrease ohmic heating demand, however, and this reduces the overall thermal input, increasing efficiency. The change in overall hydrogen production efficiency, however, was less than ±0.1% for a ±20°C change in recuperator approach temperature limits. The
efficiency of the product heaters, therefore, is found to be insignificantly related to the overall hydrogen production efficiency. Additionally, this heat is small enough that it is provided by the steam turbine for the separate water boiler loops integration scheme.

5.4.3. HTSE Overpotential

The overpotential of the HTSE directly influences the hydrogen production efficiency, with little impact on the hydrogen production rate. The highest

![Graph showing hydrogen production efficiency as a function of overpotential](image)

Figure 5.4: Hydrogen production efficiency of GFR-HTSE as a function of overpotential
efficiency that can be attained, shown in Table 5.6, is 50.6%, represented by a zero overpotential. This optimized situation represents the ideal or reversible electrolysis of steam, with no energy losses. As the overpotential increases, with all other variables held constant, the hydrogen production efficiency decreases. This relationship is shown in Fig. 5.4.

5.4.3. Reactor Coolant Draw Fraction

The amount of heat withdrawn from the reactor was found to have the largest influence on both the hydrogen production efficiency and the hydrogen production rate.

![Figure 5.5: Hydrogen production rate as a function of reactor heat draw percentage](image-url)
according to the sensitivity analysis performed. As an increasing amount of heat is withdrawn from the reactor, a larger water boiler duty is made possible. This increased water boiler heat provides the heat needed to vaporize a larger amount of water, thus increasing the hydrogen production rate. The upper limit of this trend is reached at a flow rate of 97.6 kg/s feedwater. Above this flow rate, the heat taken from the reactor is sufficient that there is not enough electricity produced to fully electrolyze the increased steam flow. At this point, the hydrogen production rate will be limited by electricity production in the reactor, rather than steam flow rate. The relationship of hydrogen production rate and reactor heat draw is found in Fig. 5.5. As the reactor heat draw percentage decreases, the electricity demand in the HTSE unit is decreased. The difference between the electrolysis electricity demanded, and the electricity produced in
the reactor is then made available to the grid. This “excess” electricity as a function of heat draw percentage can be seen in Fig. 5.6, and it increases as the draw fraction decreases.

The other significant characteristic affected by the heat draw ratio adjustment is the overall hydrogen production efficiency. By adjusting the heat draw ratio, the relationship between the heat draw ratio and the hydrogen production efficiency was found to be an inverse proportionality as seen in Fig. 5.7. This relation provides the understanding that a balance must be found between increasing the hydrogen production rate and decreasing the overall hydrogen production efficiency. It would therefore be worthwhile to determine the optimal heat draw at which an appropriate balance between hydrogen production rate and hydrogen production efficiency can be achieved.

![Hydrogen Production Efficiency](image)

Figure 5.7: Hydrogen production efficiency as a function of the reactor heat draw percentage
5.5 Modeling and Results Summary

The process for determining a preferred layout for integration of the HTSE and the S-CO₂-GFR required modeling each setup in different programs. The resulting thermodynamic data were then utilized in MathCAD to calculate the properties of each layout. By following this procedure, the hydrogen flow rate, the heat requirements, and the process efficiencies could be determined. These same values were calculated using a very similar process by the INL. This process differed in layout construction due to the fact that the INL scientists had incorporated hydrogen in the feed stream, and steam in the product stream to prevent dryout. In addition, the properties of the HTSE were slightly different due to the use of an accurate 1-D HTSE flow model in the INL calculations. The INL results include the same values as MIT’s results, but they also contain the properties of the HTSE stack, as calculated from the 1-D model. The resulting data from INL was then compared to the data from this thesis, and found to be in good agreement.

A sensitivity analysis was also performed on the major process variables of the GFR-HTSE plant to determine which variables influence the hydrogen production rate and hydrogen production efficiencies the most. The heat draw percentage and the overpotential value most influence the hydrogen production efficiency. For both cases, an increase in the given variables decreases the hydrogen production rate, with the overpotential being a greater influence. The heat draw fraction and the product temperatures most directly influence the hydrogen production rate. The hydrogen production rate is increased by a decrease in product temperatures and by an increase in
the heat draw fraction. The hydrogen production rate is more strongly influenced by the heat draw fraction, but there is a limit to increasing the hydrogen production rate by this variable; this limit is reached when the electricity produced by the GFR-PCS is no longer sufficient to electrolyze the entire steam flow.
Chapter 6 Conclusions and Final Remarks

6.1 Summary and Conclusions

Hydrogen has great potential to become a crucial component in several global energy plans. Currently, hydrogen is produced via methane reforming, but it should be possible to reduce CO₂ emissions and production costs if hydrogen were produced using nuclear energy. Several methods for producing nuclear hydrogen have been proposed, including High Temperature Steam Electrolysis, the Sulfur-Iodine process, and nuclear-assisted methane reforming. Each of these processes uses heat and/or electricity from a nuclear reactor to assist in the hydrogen production process. In this work, due to its more mature state of development and applicability to other reactors in addition to the high temperature reactor, plus its high efficiency, the HTSE process has been selected as the process to investigate.

The primary candidates for a nuclear reactor for the production of nuclear hydrogen are helium-cooled thermal spectrum very high temperature reactors (VHTR) and gas-cooled fast reactors (GFR) due to the high temperatures of the coolant leaving the reactor core. Thus such reactors can be coupled directly to thermochemical plants, or produce electricity for HTSE at high efficiency. In the NERI project which supported the present study, the approach is to employ a GFR powering a supercritical CO₂ power conversion system. This operates at much lower temperatures (≤650°C) but at comparable efficiencies. Hence while unsuitable for the thermochemical approach, it is a
prime candidate for HTSE service. For this reason, the S-CO₂-GFR has been selected for this thesis as the reactor of choice for nuclear hydrogen production.

Prior work at MIT has evaluated the concept of coupling gas cooled reactors with the HTSE process [3.1][3.2]. The present work builds upon this earlier concept, and focuses on optimizing the integration of the HTSE plant with the nuclear reactor. Several methods were investigated using ASPEN to determine the optimal integration of the HTSE plant and the S-CO₂-GFR. Two methods of integration were found to be the most promising: the extraction of PCS turbine exhaust to boil water in an IHX, or the extraction of coolant directly from the GFR to boil water in an IHX. These two studies analyzed thermodynamics, safety issues, and material constraints. The extraction of turbine exhaust is slightly more efficient, but may have unintended negative effects on the overall process, as the PCS is influenced strongly by extraction from this point. The direct extraction of coolant from the reactor is of comparable efficiency, but has the added benefits of serving as a constantly running ECS/SCS. Furthermore, the PCS performance and controls are not affected when coolant is extracted from reactor itself. This thesis is therefore based upon the design extracting coolant from the reactor directly. This integrated plant is then improved further by maximizing the thermal recuperation of the cycle. A preheater has been added to heat the feedwater to 82°C, and the product streams are used to heat the post IHX steam to nearly 870°C. This drastically reduces the required nuclear heat demand in the integrated plant for hydrogen production.

Several models of HTSE cells have been developed. The first is a simple overpotential model, in which the “efficiency” of the HTSE cell is considered to be the ratio of the realistic energy required for electrolysis divided by the ideal energy required.
This difference between the ideal energy and the actual energy required for electrolysis is called the overpotential, and a 10% value is used to model the HTSE cells. The INL has developed more in-depth models that determine exact conditions required in the HTSE electrolytic cell in order for hydrogen production to occur, as well as the hydrogen production rate.

The integration of the HTSE plant and the 2400 MW<sub>th</sub> S-CO<sub>2</sub>-GFR as described in chapter 3 has been identified as the optimal integration, as the hydrogen production rate is nearly 10.4 kg/s, or nearly 300,000 scf of hydrogen per day. The efficiency for hydrogen production (which is defined as the energy value of the hydrogen, or the lower heating value of hydrogen, divided by the thermal energy required to produce the hydrogen) is approximately 47.3%. The INL has also prepared a layout integrating the HTSE plant which they have modeled using the 1-D MathCAD model with the Helium Cooled GFR. Their model incorporates hydrogen in the HTSE feed stream, and steam in the product stream to prevent dryout of the HTSE electrodes. Even with this difference, the INL results provide a close benchmark for the results reached in this thesis; the H<sub>2</sub> production per MW<sub>e</sub> agrees within 5%. From this data, 4 primary conclusions have been determined:

1. The optimal mode of integration of a GFR and an HTSE plant is to extract coolant directly from the reactor to boil water in an IHX. This process has a comparable efficiency to the extraction of the coolant from the PCS turbine exhaust, but there are two primary benefits which make it more desirable: an inherent safety feature due to having constant heat removal (9.2%) from the
reactor, self-powered by a separate electricity source; and there is no disruption of the PCS by extraction of coolant in the middle of the cycle.

2. A S-CO$_2$-GFR can compete with a Helium cooled GFR in terms of efficiency and hydrogen production rates. The S-CO$_2$-GFR has less stringent material constraints, as the reactor outlet temperature ranges between 550°C and 750°C, which is significantly less than the helium cooled GFR outlet temperature (850°C). The S-CO$_2$-GFR power conversion system is also more compact.

3. Because of the high thermal recuperation that has been achieved in the HTSE plant layout here described, any nuclear reactor can be used to supply heat to a hydrogen production plant. The highest quality heat (required at temperatures above 273°C) is supplied by recuperation from the product H$_2$ and O$_2$ streams, and is therefore independent of the reactor used. Since modern day reactors have outlet temperatures greater than 273°C, any reactor can fulfill this requirement.

4. Although any reactor can satisfy the thermal requirement of hydrogen production via HTSE, the S-CO$_2$-GFR is still more desirable because of its high efficiency. The overall process hydrogen efficiency is dependant upon the thermodynamic heat-to-work efficiency of the reactor PCS to which it has been connected. While a S-CO$_2$-GFR with an integrated HTSE plant would have a hydrogen production efficiency of 47.3%, a standard LWR or PWR would only have a hydrogen production efficiency of around 37.4%-40.6%.
6.2 Future Work

There are three primary areas in which future work is needed before a definitive statement can be made about the integration of HTSE with nuclear energy to produce hydrogen. Resolution of these points will greatly enhance the argument that hydrogen should be produced using a S-CO$_2$-GFR and HTSE.

1. The overpotential model in the ASPEN calculation should be replaced with a 1-D model, as has been done by the INL. This would require condensing the MathCAD model into a simple yet accurate code that could be input as a user-defined function in the HTSE cell unit in ASPEN. This would provide a more accurate value of the overpotential for electrolysis, rather than an approximate value.

2. The HTSE plant layout should be revised to prevent dryout. In order to prevent this, the INL has incorporated steam in the product stream, and hydrogen in the feed stream for the HTSE cells. A similar approach or another method should be applied to the layout provided in this thesis. By adapting the ASPEN model to account for and prevent dryout, a significantly more accurate and possibly more efficient design can be achieved to further improve the hydrogen production capacity of the S-CO$_2$-GFR-HTSE plant. Water removal from the H$_2$ stream should also be explicitly modeled. For applications where the H$_2$ and O$_2$ product streams (at 6 MPa) exceed requirements, work recovery using turbines should be evaluated.
3. An in depth economic analysis should be conducted to quantify the cost-effectiveness of producing hydrogen using this method. Though the efficiency is comparable to other methods, it should be determined whether the beginning-to-end process of producing hydrogen is one that will have a place in the economy that exists today, or will exist in the future.

4. A model which uses half of the LTR for boiling water while using higher quality heat to raise the temperature of the steam should be created. This is an appealing option which allows for using lower quality heat to boil water, while still providing a sufficient temperature to maintain the required vapor pressure of 6 MPa. Because of thermodynamic benefits, this may prove to be an even more desirable integration scheme than those presented in this thesis.
References


[4.2] Personal Communication: J. Steven Herring (Idaho National Laboratory) to Matthew J Memmott (MIT), April, 20, 2006


Reactor Thermal-Hydraulics (NURETH-11), Presented at NURETH-11, Popes Palace Conference Center, Avignon, France, October 2005.


[4.8] HYSIS®, Aspen Technology, Inc., Cambridge, MA, USA


[A.1] Personal Communication: Grant L. Hawkes (Idaho National Laboratory) by email to Matthew J Memmott (MIT), April 24, 2006
Appendix A

This appendix lists the mathCAD program code used by INL to determine the thermal-neutral operating potential and operating temperature of the HTSE unit. This model was created by Jim O'Brien, as discussed in Ref. [3.4]. In the INL calculations discussed in chapter 5, the model found below was entered into HYSIS and used as the primary parameters for the HTSE unit modeling. This was done by Grant Hawkes using numerical integration in Excel, and was sent by Grant to the author of this thesis in April, 2006 [A. 1]. (Minor revisions to this code were performed by the author of this thesis for printing purposes.)

Definitions

\[
\begin{align*}
TOL & := 0.00001 \\
CTOL & := 0.00001 \\
J_{fa} & := 96487 \frac{J}{V \cdot \text{mol}} \\
P_{std} & := 101320 \text{Pa} \\
T_{std} & := 273 \text{K} \\
R_{u} & := 8.314 \frac{J}{\text{mol} \cdot \text{K}}
\end{align*}
\]

Subscript definitions:  \( i = \text{inlet} \),  \( o = \text{outlet} \),  \( 0 = \text{H}_2\text{O} \),  \( 1 = \text{H}_2 \),  \( 2 = \text{O}_2 \),  \( 3 = \text{N}_2 \),  \( 4 = \text{Air} \)

\[
\begin{align*}
\text{H}_2\text{O} & := 0 \\
\text{H}_2 & := 1 \\
\text{O}_2 & := 2 \\
\text{N}_2 & := 3 \\
\text{AIR} & := 4 \\
j & := 0..4
\end{align*}
\]

\[
\begin{align*}
\text{MW}_{\text{H}_2\text{O}} & := 18.015 \frac{\text{gm}}{\text{mol}} \\
\text{MW}_{\text{H}_2} & := 2.016 \frac{\text{gm}}{\text{mol}} \\
\text{MW}_{\text{O}_2} & := 31.999 \frac{\text{gm}}{\text{mol}} \\
\text{MW}_{\text{N}_2} & := 28.0134 \frac{\text{gm}}{\text{mol}}
\end{align*}
\]

\[
\begin{align*}
\text{MW}_{\text{AIR}} & := 0.21 \cdot \text{MW}_{\text{O}_2} + 0.79 \cdot \text{MW}_{\text{N}_2}
\end{align*}
\]

\[
\rho_{std} := \begin{cases} 
\rho & \text{for } i \in 0..4 \\
\frac{p_{std} \cdot \text{MW}_i}{R_u \cdot T_{std}} & \text{otherwise}
\end{cases}
\]

Definitions

Input parameters on per-cell basis:

Number of cells:  \( N_{\text{cells}} := 1 \)

Cell size in cm\(^2\):  \( A_{\text{cell}} := 64 \text{cm}^2 \)

ASR:  \( ASR_{\text{fixed}} := 1.5 \text{ohm-cm}^2 \)

\( ASR_{\text{CASE}} = 0 \) for fixed value, 1 for calculated \( f(T) \):  \( ASR_{\text{CASE}} := 0 \)

Note: \( ASR(1100) = 2.308 \) corresponds to Grant's FLUENT model  \( ASR_{\text{at}_1100} := 1.5 \text{ohm-cm}^2 \)

HEAT\_CASE = 0 for adiabatic, 1 for isothermal:  \( HEAT_{\text{CASE}} := 0 \)
Reactants inlet temperature:

Inlet fuel side H2/H2O total mass flow rate:

Inlet mole fraction H2 on fuel side:

Sweep mass flow rate:

Enter sweep side inlet composition in mole fraction:

Operating pressure (Pa):

Power cycle efficiency:

From Black and Hartley, p 631:

\[ Q - W = \sum_{p} N_i [\Delta h_i^\circ + h_i(T_p) - h_i^\circ] - \sum_{p} N_i [\Delta h_i^\circ + h_i(T_R) - h_i^\circ] \]

Conversion from Mike's inputs

\[ y_{i \_ fuel \_ O2} := y_{i \_ fuel \_ O2} + 0.21 \cdot y_{i \_ fuel \_ AIR} \]

\[ y_{i \_ fuel \_ N2} := y_{i \_ fuel \_ N2} + 0.79 \cdot y_{i \_ fuel \_ AIR} \]

\[ y_{i \_ fuel \_ AIR} := 0.0 \]

\[ M_{i \_ fuel \_ total} := \frac{M_{i \_ fuel \_ total}}{N_{cells}} \]

\[ y_{i \_ sweep \_ O2} := y_{i \_ sweep \_ O2} + 0.21 \cdot y_{i \_ sweep \_ AIR} \]

\[ y_{i \_ sweep \_ N2} := y_{i \_ sweep \_ N2} + 0.79 \cdot y_{i \_ sweep \_ AIR} \]

\[ y_{i \_ sweep \_ AIR} := 0.0 \]

\[ M_{i \_ sweep \_ total} := \frac{M_{i \_ sweep \_ total}}{N_{cells}} \]

\[ T_f := 1073 \text{ K} \]

\[ M_{i \_ fuel \_ total} := 1.5813 \times 10^{-2} \text{ gm/s} \]

\[ y_{i \_ fuel \_ H2} := 0.125 \]

\[ y_{i \_ fuel \_ H2O} := 0.5 \]

\[ y_{i \_ fuel \_ O2} := 0 \]

\[ y_{i \_ fuel \_ N2} := 0.375 \]

\[ y_{i \_ fuel \_ AIR} := 0 \]

\[ M_{i \_ sweep \_ total} := 0.0648 \text{ gm/s} \]

\[ y_{i \_ sweep \_ H2O} := 0 \]

\[ y_{i \_ sweep \_ H2} := 0 \]

\[ y_{i \_ sweep \_ O2} := 0.999 \]

\[ y_{i \_ sweep \_ N2} := 0.001 \]

\[ y_{i \_ sweep \_ AIR} := 0 \]

\[ P_{atm} := 1.0134 \times 10^6 \text{ Pa} \]

\[ \eta_{power \_ cycle} := 0.45 \]
\[
\begin{align*}
\text{MW}_{i_{\text{fuel avg}}} := \sum_j (y_{i_{\text{fuel j}}} \cdot \text{MW}_j) \\
\text{MW}_{i_{\text{sweep avg}}} := \sum_j (y_{i_{\text{sweep j}}} \cdot \text{MW}_j) \\
\text{N}_{i_{\text{fuel total}}} := \frac{M_{i_{\text{fuel total}}}}{\text{MW}_{i_{\text{fuel avg}}}} \\
\text{N}_{i_{\text{sweep total}}} := \frac{M_{i_{\text{sweep total}}}}{\text{MW}_{i_{\text{sweep avg}}}}
\end{align*}
\]

Conversion from Mike's inputs

- Fit enthalpy data

de\text{Data}=

<table>
<thead>
<tr>
<th>T (K)</th>
<th>(h_{\text{H}_2\text{O}}) (J/mol)</th>
<th>(s_{\text{H}_2\text{O}}) (J/mol K)</th>
<th>(h_{\text{H}_2}) (J/mol)</th>
<th>(s_{\text{H}_2}) (J/mol K)</th>
<th>(h_{\text{O}_2}) (J/mol)</th>
<th>(s_{\text{O}_2}) (J/mol K)</th>
<th>(h_{\text{N}_2}) (J/mol)</th>
<th>(s_{\text{N}_2}) (J/mol K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>298</td>
<td>9904</td>
<td>188.72</td>
<td>8468</td>
<td>130.57</td>
<td>8682</td>
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\[ \Delta h_{f_{\text{H}_2O}} := -241820 \frac{J}{mol} \]  
standard state enthalpy of formation for H2O

\[ \Delta h_{f_{\text{H}_2}} := 0 \frac{J}{mol} \]  
standard state enthalpy of formation for H2

\[ \Delta h_{f_{\text{O}_2}} := 0 \frac{J}{mol} \]  
standard state enthalpy of formation for O2

\[ \Delta h_{f_{\text{N}_2}} := 0 \frac{J}{mol} \]  
standard state enthalpy of formation for N2

\[ \Delta h_{f_{\text{AIR}}} := 0 \frac{J}{mol} \]  
standard state enthalpy of formation for AIR

\[ \Delta H_R(T) := \left(2.9359 \times 10^5 - 3.7916 \times 10^4 \cdot T^{-3} + 1.2982 \times 10^4 \cdot T^{-5} - 1.2317 \times 10^3 \cdot T^{-7}\right) \frac{J}{mol} \]

\[ T := \text{thdata} \]  
\[ T := T \cdot 1 - K \]  
\[ \text{HHV} := 285830 \frac{J}{mol} \]  
\[ \text{LHV} := -\Delta h_{f_{\text{H}_2O}} \]

\[ h := \text{for } i \in 0..3 \]
\[ h_1 := \text{thdata} \left(2+1\right) \frac{J}{mol} \]
\[ h \]

\[ h_4 := \left(0.21 \cdot \text{thdata} \left(5\right) + 0.79 \cdot \text{thdata} \left(7\right)\right) \frac{J}{mol} \]

\[ F(x) := \begin{pmatrix}
1 \\
x \\
x^2 \\
x^3
\end{pmatrix} \]

\[ h_{\text{fit}}(T_p) := \text{for } i \in 0..4 \]
\[ v_i := \text{linfit} \left(\frac{T}{K}, \frac{h_i}{J/mol}, F\right) \frac{J}{mol} \]
\[ \text{temp}_i := v_i \cdot F(T_p) \]
\[ \text{temp} \]

\[ TT := 1073 \]

\[ h_{\text{fit}}(TT)_{\text{O}_2} = \frac{J}{mol} \]
\[ h_{\text{fit}(TT)H_2O} = \frac{J}{\text{mol}} \quad h_{\text{fit}(TT)H_2} = \frac{J}{\text{mol}} \quad h_{\text{fit}(TT)N_2} = \frac{J}{\text{mol}} \]

\[ V_{\text{th}}(T) := \begin{cases} 2.935910^5 - 3.7916110^4 \left( \frac{T}{K} \right)^{0.3} + 1.2982110^4 \left( \frac{T}{K} \right)^{0.5} - 1.231710^3 \left( \frac{T}{K} \right)^{0.7} \end{cases} \frac{J}{\text{mol}} \]

Fit enthalpy data

Main Program

Calculate per-cell current:

Calculate hydrogen production rate:

Electrolyze =

\[ I \leftarrow i \cdot A_{\text{cell}} \]

\[ \Delta N_{H_2} \leftarrow \frac{I}{2 \cdot F_a} \]

\[ N_{i_{\text{fuel total}}} \leftarrow N_{i_{\text{fuel_total}}} \]

\[ y_{i_{\text{fuel_H}_2}} \leftarrow y_{i_{\text{fuel_H}_2}} \cdot N_{i_{\text{fuel_total}}} + \Delta N_{H_2} \]

\[ y_{i_{\text{fuel_H}_2O}} \leftarrow \frac{y_{i_{\text{fuel_H}_2}} \cdot N_{i_{\text{fuel_total}}} - \Delta N_{H_2}}{N_{i_{\text{fuel_total}}} - \Delta N_{H_2}} \]

\[ y_{i_{\text{fuel_O}_2}} \leftarrow \frac{y_{i_{\text{fuel_O}_2}} \cdot N_{i_{\text{fuel_total}}} - \Delta N_{H_2}}{N_{i_{\text{fuel_total}}} - \Delta N_{H_2}} \]

\[ y_{i_{\text{fuel_N}_2}} \leftarrow \frac{y_{i_{\text{fuel_N}_2}} \cdot N_{i_{\text{fuel_total}}} - \Delta N_{H_2}}{N_{i_{\text{fuel_total}}} - \Delta N_{H_2}} \]

\[ y_{i_{\text{fuel_AIR}}} \leftarrow 0.0 \]

\[ M_{i_{\text{fuel_total}}} \leftarrow N_{i_{\text{fuel_total}}} \sum_{j} y_{i_{\text{fuel_j}}} \cdot MW_j \]

\[ N_{i_{\text{sweep_total}}} \leftarrow N_{i_{\text{sweep_total}}} + \frac{\Delta N_{H_2}}{2} \]

\[ y_{i_{\text{sweep_H}_2O}} \leftarrow \frac{y_{i_{\text{sweep_H}_2O}} \cdot N_{i_{\text{sweep_total}}} + 2}{N_{i_{\text{sweep_total}}} + 2} \]

\[ y_{i_{\text{sweep_H}_2}} \leftarrow \frac{y_{i_{\text{sweep_H}_2}} \cdot N_{i_{\text{sweep_total}}}}{N_{i_{\text{sweep_total}}}} \]
\[
\begin{align*}
\frac{y_{\text{o\_sweep\_O}_2}}{N_{\text{o\_sweep\_total}}} &= \frac{y_{\text{i\_sweep\_O}_2} \cdot N_{\text{i\_sweep\_total}} + \frac{\Delta N_{\text{H}_2}}{2}}{N_{\text{o\_sweep\_total}}} \\
\frac{y_{\text{o\_sweep\_N}_2}}{N_{\text{o\_sweep\_total}}} &= \frac{y_{\text{i\_sweep\_N}_2} \cdot N_{\text{i\_sweep\_total}}}{N_{\text{o\_sweep\_total}}} \\
y_{\text{o\_sweep\_AIR}} &= 0.0 \\
M_{\text{o\_sweep\_total}} &= N_{\text{o\_sweep\_total}} \sum_j (y_{\text{o\_sweep\_j}} \cdot MW_j) \\
\text{Mass Balance} &= M_{\text{o\_fuel\_total}} + M_{\text{o\_sweep\_total}} - M_{\text{i\_fuel\_total}} \\
&\quad + -M_{\text{i\_sweep\_total}} \\
H_{\text{i\_fuel}} &= N_{\text{i\_fuel\_total}} \sum_j \left( y_{\text{i\_fuel\_j}} \left( \Delta h_f_j + h_{\text{fit}} \left( \frac{T_r}{K} \right)_j - h_{\text{fit}(298)j} \right) \right) \\
H_{\text{i\_sweep}} &= N_{\text{i\_sweep\_total}} \sum_j \left( y_{\text{i\_sweep\_j}} \left( \Delta h_f_j \left( h_{\text{fit}} \left( \frac{T_r}{K} \right)_j \right) \right) - h_{\text{fit}(298)j} \right) \\
H_{\text{o\_fuel}(T_p)} &= N_{\text{o\_fuel\_total}} \sum_j \left( y_{\text{o\_fuel\_j}} \left( \Delta h_f_j \left( h_{\text{fit}} \left( \frac{T_p}{K} \right)_j \right) \right) + h_{\text{fit}(298)j} \right) \\
H_{\text{o\_sweep}(T_p)} &= N_{\text{o\_sweep\_total}} \sum_j \left( y_{\text{o\_sweep\_j}} \left( \Delta h_f_j \left( h_{\text{fit}} \left( \frac{T_p}{K} \right)_j \right) \right) - h_{\text{fit}(298)j} \right) \\
A_1 &= -238.241 \\
A_2 &= -0.0399522 \\
A_3 &= -3.31866 \times 10^{-6} \\
A_4 &= -3.53216 \times 10^{-11} \\
A_5 &= 0.0128498 \\
\Delta G(T) &= (A_1 + A_2 \cdot T + A_3 \cdot T^2 + A_4 \cdot T^3 + A_5 \cdot T \cdot \ln(T)) \cdot 1000 \cdot \frac{J}{\text{mol}} \\
\text{if} \quad \text{HEAT\_CASE} = 0 \quad \text{then} \quad \text{else} \\
A &= \frac{1}{-2 \times a_1 \cdot (T - T_p) \cdot (y_{\text{o\_fuel\_H}_2} - y_{\text{i\_fuel\_H}_2}) \cdot (y_{\text{o\_sweep\_O}_2} - y_{\text{i\_sweep\_O}_2})} \\
B &= \Delta G \left( \frac{T}{K} \right) + R \cdot u \cdot T \cdot \ln \left[ \frac{1 - y_{\text{H}_2} - y_{\text{i\_fuel\_N}_2} - y_{\text{i\_fuel\_AIR}}}{y_{\text{H}_2} \cdot y_{\text{O}_2} \cdot \left( \frac{P_{\text{atm}}}{P_{\text{std}}} \right)^5} \right]
\end{align*}
\]
\[
V_{\text{Nemst}}(T_p) = -1 \cdot \left( \int_{T_r}^{T_p} y_{o\text{-sweepO}_2} dy_{o\text{-fuelH}_2} + \int_{T_r}^{T_p} y_{i\text{-sweepO}_2} dy_{i\text{-fuelH}_2} \right) + A \cdot B \cdot dy_{H_2} dy_{O_2} dT
\]

\[
C = \int_{T_r}^{T_p} \left( \frac{ASR_{\text{at 1100}}}{\text{ohm-cm}^2} - 0.463 \right) + 3.973 \cdot 10^{-5} \cdot \exp \left( \frac{10300}{T} \right) dT
\]

\[
\text{ASR}(T_p) = \begin{cases} 
\text{if ASR_CASE = 0, ASR fixed:} & \left( \frac{1}{T_p - T_r} \right) \cdot \text{ohm-cm}^2 \\
\text{otherwise} & \end{cases}
\]

\[
V_{\text{op}}(T_p) = i \cdot \text{ASR}(T_p) + V_{\text{Nemst}}(T_p)
\]

\[
\text{Work}(T_p) = -V_{\text{op}}(T_p) \cdot I
\]

\[
Q_{\text{added}}(T_p) = 0.0
\]

\[
Q(T_p) = \text{Work}(T_p) + H_{o\text{-fuel}}(T_p) + H_{o\text{-sweep}}(T_p) - H_{i\text{-fuel}} - H_{i\text{-sweep}} - Q_{\text{added}}(T_p)
\]

\[
T_p \leftarrow 1000 \text{ K}
\]

\[
T_{p\text{ converged}} \leftarrow \text{root}(Q(T_p), T_p)
\]

\[
G = \frac{1}{2 \cdot F_a \left( y_{o\text{-fuelH}_2} - y_{i\text{-fuelH}_2} \right) \left( y_{o\text{-sweepO}_2} - y_{i\text{-sweepO}_2} \right)}
\]

\[
F = \Delta G \left( \frac{T_p}{K} \right) + R_u \cdot T_p \cdot \ln \left[ 1 - \frac{y_{H_2} - y_{i\text{-fuelN}_2} - y_{i\text{-fuelAIR}}}{y_{H_2} y_{O_2} \left( \frac{p_{\text{atm}}}{p_{\text{std}}} \right)^{5}} \right]
\]

\[
V_{\text{Nemst}}(T_p) = -1 \cdot \left( \int_{T_r}^{T_p} y_{o\text{-sweepO}_2} dy_{o\text{-fuelH}_2} + \int_{T_r}^{T_p} y_{i\text{-sweepO}_2} dy_{i\text{-fuelH}_2} \right) + G \cdot F \cdot dy_{H_2} dy_{O_2}
\]

\[
\text{ASR}(T_p) = \begin{cases} 
\text{if ASR_CASE = 0, ASR fixed:} & \left[ \frac{ASR_{\text{at 1100}}}{\text{ohm-cm}^2} - 0.463 \right] \cdot \text{ohm-cm}^2 \\
\text{otherwise} & \end{cases}
\]

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\[ V_{op}(T_p) \leftarrow i \cdot ASR(T_p) + V_{Nernst}(T_p) \]
\[ \text{Work}(T_p) \leftarrow -V_{op}(T_p) \cdot l \]
\[ Q_{added}(T_p) \leftarrow l \cdot (V_{tn}(T_p) - V_{op}(T_p)) \]
\[ Q(T_p) \leftarrow \text{Work}(T_p) + H_{o.fuel}(T_p) + H_{o.sweep}(T_p) - H_{i.fuel} - H_{i.sweep} - Q_{added}(T_p) \]
\[ T_p \leftarrow T_r \]
\[ T_{p\_converged} \leftarrow T_r \]
\[ R_0 \leftarrow \frac{i \cdot cm^2}{A} \]
\[ R_1 \leftarrow \frac{ASR(T_{p\_converged})}{\text{ohm} \cdot \text{cm}^2} \]
\[ R_2 \leftarrow \frac{V_{op}(T_{p\_converged})}{V} \]
\[ R_3 \leftarrow \frac{V_{Nernst}(T_{p\_converged})}{V} \]
\[ R_4 \leftarrow \frac{T_{p\_converged}}{K} \]
\[ R_5 \leftarrow \frac{Q_{added}(T_{p\_converged}) \cdot N_{\text{cells}}}{\text{kW}} \]
\[ R_6 \leftarrow \frac{\text{Work}(T_{p\_converged}) \cdot N_{\text{cells}}}{W} \]
\[ R_7 \leftarrow \frac{Q_{added}(T_{p\_converged})}{Q_{added}(T_{p\_converged}) \cdot \text{Work}(T_{p\_converged})} \]
\[ R_8 \leftarrow \text{Mass Balance} \cdot N_{\text{cells}} \cdot \text{hr} \cdot \text{kg} \]
\[ R_9 \leftarrow \frac{Q(T_{p\_converged}) \cdot N_{\text{cells}}}{\text{kW}} \]

for \( j \in 0..4 \)
\[ R_{10+j} \leftarrow y_{i.fuel_j} \]
\[ R_{15+j} \leftarrow y_{o.fuel_j} \]
\[ R_{20+j} \leftarrow y_{i.sweep_j} \]
\[ R_{25+j} \leftarrow y_{o.sweep_j} \]
\begin{align*}
R_{30} & \leftarrow \frac{H_i_{\text{fuel}}}{W} \\
R_{31} & \leftarrow \frac{H_i_{\text{sweep}}}{W} \\
R_{32} & \leftarrow \frac{H_{o_{\text{fuel}}}(T_{p_{\text{converged}}})}{W} \\
R_{33} & \leftarrow \frac{H_{o_{\text{sweep}}}(T_{p_{\text{converged}}})}{W} \\
\end{align*}

\textbf{Main Program}

\texttt{Enter number of values (integer): } N := 10

\texttt{Current\_Density\_Array} = \begin{pmatrix}
0.001 \\
0.025 \\
0.05 \\
0.075 \\
0.1 \\
0.15 \\
0.2 \\
0.25 \\
0.3 \\
0.35 \\
0.4 \\
\end{pmatrix} \ \text{A cm}^{-2}

\texttt{Run Program}

\texttt{Z := for i \in 0..N}

\texttt{ii \leftarrow Current\_Density\_Array}

\texttt{Z[j] \leftarrow ELECTROLYZ[z]}

\texttt{Z^T}

\texttt{Run Program}
Define output variables

Returned data subscripts: 0 = i (A/cm²), 1 = ASR (ohm-cm²), 2 = V_op, 3 = V_Nernst, 4 = T_converged, 5 = Q_added, 6 = Work (kW), 7 = Q_added/(Q_added + Work), 8 = Mass Balance Error, 9 = Heat Balance Error

\[ y_i_{\text{fuel AIR}} = \begin{cases} 10 = y_{i_{\text{fuel H2O}}} & 11 = y_{i_{\text{fuel H2}}} & 12 = y_{i_{\text{fuel O2}}} & 13 = y_{i_{\text{fuel N2}}} & 14 = y_{i_{\text{fuel AIR}}} \\ 15 = y_{o_{\text{fuel H2O}}} & 16 = y_{o_{\text{fuel H2}}} & 17 = y_{o_{\text{fuel O2}}} & 18 = y_{o_{\text{fuel N2}}} & 19 = y_{o_{\text{fuel AIR}}} \\ 20 = y_{i_{\text{sweep H2O}}} & 21 = y_{i_{\text{sweep H2}}} & 22 = y_{i_{\text{sweep O2}}} & 23 = y_{i_{\text{sweep N2}}} & 24 = y_{i_{\text{sweep AIR}}} \\ 25 = y_{o_{\text{sweep H2O}}} & 26 = y_{o_{\text{sweep H2}}} & 27 = y_{o_{\text{sweep O2}}} & 28 = y_{o_{\text{sweep N2}}} & 29 = y_{o_{\text{sweep AIR}}} \\ \end{cases} \]

\[
\begin{align*}
\text{i} & := Z^{(1)} \cdot \frac{A}{cm^2} \\
\text{ASR} & := Z^{(1)} \cdot \text{ohm-cm}^2 \\
\text{V_op} & := Z^{(2)} \cdot V \\
\text{V_Nernst} & := Z^{(3)} \cdot V \\
y_{i_{\text{sweep H2O}}} & := Z^{(20)} \\
y_{o_{\text{sweep H2O}}} & := Z^{(25)} \\
y_{i_{\text{sweep H2}}} & := Z^{(21)} \\
y_{o_{\text{sweep H2}}} & := Z^{(26)} \\
y_{i_{\text{sweep O2}}} & := Z^{(22)} \\
y_{o_{\text{sweep O2}}} & := Z^{(27)} \\
y_{i_{\text{sweep N2}}} & := Z^{(23)} \\
y_{o_{\text{sweep N2}}} & := Z^{(28)} \\
y_{i_{\text{sweep AIR}}} & := Z^{(24)} \\
y_{o_{\text{sweep AIR}}} & := Z^{(29)} \\
\end{align*}
\]
\[ T_{\text{converged}} := Z^{(4)} \cdot K \]
\[ Q_{\text{added}} := Z^{(5)} \cdot kW \]
\[ \text{Work} := Z^{(6)} \cdot kW \]
\[ \text{Power Ratio} := Z^{(7)} \]

\[ \eta_{\text{ideal overall}} := \frac{i \cdot A_{\text{cell}} \cdot N_{\text{cells}} \cdot \text{LHV}}{2 \cdot Fa} \]

\[ \eta_{\text{ideal overall \_ AHR}} := \frac{i \cdot A_{\text{cell}} \cdot N_{\text{cells}} \cdot \text{AHR}}{2 \cdot Fa} \]

\[ \eta_{\text{LHV}} := \frac{\text{LHV}}{V_{\text{op}} \cdot 2 \cdot Fa} \]
\[ \eta_{\text{HHV}} := \frac{\text{HHV}}{V_{\text{op}} \cdot 2 \cdot Fa} \]

\[ \text{Mass Balance Error} := Z^{(8)} \cdot \frac{\text{kg}}{hr} \]
\[ \text{Heat Balance Error} := Z^{(9)} \cdot kW \]

\[ Z_{\text{aug}} := \begin{array}{l}
\text{for } i \in 0..7 \\
Z_{\text{aug}}^{(i)} \leftarrow Z^{(i)} \\
Z_{\text{aug}}^{(8)} \leftarrow \eta_{\text{ideal overall}} \\
Z_{\text{aug}}^{(9)} \leftarrow \eta_{\text{ideal overall \_ AHR}} \\
Z_{\text{aug}}^{(10)} \leftarrow \eta_{\text{LHV}} \\
\text{for } i \in 8..33 \\
Z_{\text{aug}}^{(i+3)} \leftarrow Z^{(i)} \\
Z_{\text{aug}} \end{array} \]

Define output variables.
Appendix B

The following appendix contains the model created at MIT by the author of this thesis using ASPEN [A.2]. The appendix is divided into three sections: the Input Summary, in which the input parameters for the ASPEN run are described (Pages 120-123), the Run History, in which the procedures of the modeling run are detailed (Pages 124-169), and the Model Report, which indicates the convergence status for the run, the stream properties throughout the run, and the individual block properties throughout the run (Pages 169-191). The ASPEN run described by this appendix is for the “separate water boiler loops” integration method described in chapter 3 of this thesis.

**Input Summary**

; ; Input Summary created by Aspen Plus Rel. 12.1 at 11:17:57 Fri Sep 22, 2006 ; Directory H:\ Filename C:\DOCUME~1\mjm82\LOCALS~1\Temp\~apf3.tmp ;

IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='MMkcal/hr' & HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C & VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' & MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' & MASS-ENTHALP='kcal/kg' HEAT=MMkcal MOLE-CONC='mol/l' & PDROP=bar

DEF-STREAMS CONVEN ALL

DESCRIPTION "

General Simulation with Metric Units:

C, bar, kg/hr, kmol/hr, MMKcal/hr, cum/hr.

Property Method: None

Flow basis for input: Mole

Stream report composition: Mole flow"

DATABANKS PURE12 / AQUEOUS / SOLIDS / INORGANIC / & NOASPENPCD

PROP-SOURCES PURE12 / AQUEOUS / SOLIDS / INORGANIC

133
COMPONENTS
  CARBO-01 CO2 /
  WATER H2O /
  HYDRO-01 H2 /
  OXYGE-01 O2

FLOWSHEET
  BLOCK REACTOR IN=RIN OUT=ROUT
  BLOCK B2 IN=ROUT FEEDH20 OUT=RIN 1
  BLOCK B3 IN=2 OUT=5 7
  BLOCK B4 IN=11 5 OUT=O2 6
  BLOCK B5 IN=13 7 OUT=H2 8
  BLOCK B6 IN=6 8 OUT=9
  BLOCK B7 IN=15 OUT=10
  BLOCK B8 IN=10 OUT=11 13
  BLOCK B9 IN=9 OUT=15
  BLOCK B11 IN=O2 H2 OUT=14
  BLOCK B12 IN=14 17 OUT=16 FEEDH20
  BLOCK B1 IN=1 OUT=2

PROPERTIES RKS-BM
  PROPERTIES PR-BM

STREAM 17
  SUBSTREAM MIXED TEMP=20. PRES=1. MASS-FLOW=93. <kg/sec>
  MASS-FRAC WATER 1.

STREAM FEEDH20
  SUBSTREAM MIXED TEMP=30. PRES=1. MASS-FLOW=93. <kg/sec> &
  FREE-WATER=NO NPHASE=1 PHASE=L
  MASS-FRAC WATER 1.

STREAM RIN
  SUBSTREAM MIXED TEMP=489.2817 PRES=200. &
  MASS-FLOW=1143.152 <kg/sec>
  MASS-FRAC CARBO-01 1.

STREAM ROUT
  SUBSTREAM MIXED TEMP=650. PRES=200. &
  MASS-FLOW=1143.152 <kg/sec>
  MASS-FRAC CARBO-01 1.

BLOCK B6 MIXER
  PARAM PRES=60. NPHASE=1 PHASE=V T-EST=870.
  BLOCK-OPTION FREE-WATER=NO
BLOCK B11 MIXER
  PARAM PRES=60. NPHASE=1 PHASE=V T-EST=300.
  BLOCK-OPTION FREE-WATER=NO

BLOCK B3 FSPLIT
  PARAM PRES=60. NPHASE=1 PHASE=V
  FRAC 5 0.3653
  BLOCK-OPTION FREE-WATER=NO

BLOCK B8 SEP
  FRAC STREAM=11 SUBSTREAM=MIXED COMPS=OXYGE-01 FRACS=1.

BLOCK B9 HEATER
  PARAM TEMP=900. PRES=60.

BLOCK REACTOR HEATER
  PARAM PRES=200. DUTY=234.6 <MW>

BLOCK B2 HEATX
  PARAM DUTY=234.6 <MW> PRES-COLD=163. U-OPTION=PHASE &
  F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
  FEEDS HOT=ROUT COLD=FEEDH20
  PRODUCTS HOT=RIN COLD=1
  HOT-SIDE DP-OPTION=CONSTANT
  COLD-SIDE DP-OPTION=CONSTANT

BLOCK B4 HEATX
  PARAM T-COLD=870. U-OPTION=PHASE F-OPTION=CONSTANT &
  CALC-METHOD=SHORTCUT
  FEEDS HOT=11 COLD=5
  PRODUCTS HOT=O2 COLD=6
  HOT-SIDE DP-OPTION=CONSTANT
  COLD-SIDE DP-OPTION=CONSTANT

BLOCK B5 HEATX
  PARAM T-COLD=870. MIN-TAPP=5. U-OPTION=PHASE &
  F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
  FEEDS HOT=13 COLD=7
  PRODUCTS HOT=H2 COLD=8
  HOT-SIDE DP-OPTION=CONSTANT
  COLD-SIDE DP-OPTION=CONSTANT

BLOCK B12 HEATX
  PARAM T-HOT=130. PRES-COLD=2. U-OPTION=PHASE &
  F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
FEEDS HOT=14 COLD=17
PRODUCTS HOT=16 COLD=FEEDH2O
HOT-SIDE DP-OPTION=CONSTANT
COLD-SIDE DP-OPTION=CONSTANT

BLOCK B7 RSTOIC
  PARAM TEMP=900. PRES=60. HEAT-OF-REAC=NO
  STOIC 1 MIXED WATER -1. / OXYGE-01 0.5 / HYDRO-01 1.
  CONV 1 MIXED WATER 1.

BLOCK B1 COMPR
  PARAM TYPE=ISENTROPIC PRATIO=0.368098 SEFF=0.9 NPHASE=1
  BLOCK-OPTION FREE-WATER=NO

EO-CONV-OPTI

STREAM-REPOR MOLEFLOW MASSFLOW

PROPERTY-REP NOPARAM-PLUS
  ;
  ;
  ;
  ;
  ;
>>CURRENT RUN

ORIGINAL RUN APRIL 18, 2006
1:07:34 P.M. TUESDAY
INPUT FILE: _0514dku.inm
RUN ID : _0514dku

1 ;
2 ;Input file created by Aspen Plus Rel. 12.1 at 13:07:34 Tue Apr 18, 2006
3 ;Directory H:\ Runid HTSE BASE H2 ONLY 650C
4 ;
5
6
7 IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='MMkcal/hr' &
8 HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &
9 VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum'
10 &
11 MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
12 MASS-ENTHALP='kcal/kg' HEAT=MMkcal MOLE-CONC='mol/l' &
13 PDROP=bar
14
15 DEF-STREAMS CONVEN ALL
16
17 DESCRIPTION "
18 General Simulation with Metric Units :
19 C, bar, kg/hr, kmol/hr, MMKcal/hr, cum/hr.
Property Method: None
Flow basis for input: Mole
Stream report composition: Mole flow

DATABANKS PURE12 / AQUEOUS / SOLIDS / INORGANIC / & NOASPNPCD
PROP-SOURCES PURE12 / AQUEOUS / SOLIDS / INORGANIC
COMPONENTS
CARBO-01 CO2 / WATER H2O / HYDRO-01 H2 / OXYGE-01 O2

FLOWSHEET
BLOCK REACTOR IN=RIN OUT=ROUT
BLOCK B2 IN=ROUT FEEDH20 OUT=RIN 1
BLOCK B3 IN=2 OUT=5 7
BLOCK B4 IN=11 5 OUT=O2 6
BLOCK B5 IN=13 7 OUT=H2 8
BLOCK B6 IN=6 8 OUT=9
BLOCK B7 IN=15 OUT=10
BLOCK B8 IN=10 OUT=11 13
BLOCK B9 IN=9 OUT=15
BLOCK B11 IN=O2 H2 OUT=14
BLOCK B12 IN=14 17 OUT=16 FEEDH20
BLOCK B1 IN=1 OUT=2

PROPERTIES RKS-BM
PROPERTIES PR-BM

STREAM 17
SUBSTREAM MIXED TEMP=20. PRES=1. MASS-FLOW=50. <kg/sec>
MASS-FRAC WATER 1.

STREAM FEEDH20
SUBSTREAM MIXED TEMP=30. PRES=1. MASS-FLOW=50. <kg/sec> &
FREE-WATER=NO NPHASE=1 PHASE=L
MASS-FRAC WATER 1.

STREAM RIN
66  SUBSTREAM MIXED TEMP=489.2817 PRES=200. &
67       MASS-FLOW=645.3339 <kg/sec>
68  MASS-FRAC CARBO-01 1.
69
70  STREAM ROUT
71  SUBSTREAM MIXED TEMP=650. PRES=200. &
72       MASS-FLOW=645.3339 <kg/sec>
73  MASS-FRAC CARBO-01 1.
74
75  BLOCK B6 MIXER
76   PARAM PRES=60. NPHASE=1 PHASE=V T-EST=870.
77   BLOCK-OPTION FREE-WATER=NO
78
79  BLOCK B11 MIXER
80   PARAM PRES=60. NPHASE=1 PHASE=V T-EST=300.
81   BLOCK-OPTION FREE-WATER=NO
82
83  BLOCK B3 FSPLIT
84   PARAM PRES=60. NPHASE=1 PHASE=V
85   FRAC 5 0.3653
86   BLOCK-OPTION FREE-WATER=NO
87
88  BLOCK B8 SEP
89   FRAC STREAM=11 SUBSTREAM=MIXED COMPS=OXYGE-01
FRACS=1.
90
91  BLOCK B9 HEATER
92   PARAM TEMP=900. PRES=60.
93
94  BLOCK REACTOR HEATER
95   PARAM PRES=200. DUTY=129.6 <MW>
96
97  BLOCK B2 HEATX
98   PARAM DUTY=129.6 <MW> PRES-COLD=163. U-OPTION=PHASE &
99       F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
100  FEEDS HOT=ROUT COLD=FEEDH20
101  PRODUCTS HOT=RIN COLD=1
102  HOT-SIDE DP-OPTION=CONSTANT
103  COLD-SIDE DP-OPTION=CONSTANT
104
105  BLOCK B4 HEATX
106   PARAM T-COLD=870. U-OPTION=PHASE F-OPTION=CONSTANT &
107       CALC-METHOD=SHORTCUT
108   FEEDS HOT=11 COLD=5
109   PRODUCTS HOT=O2 COLD=6
110   HOT-SIDE DP-OPTION=CONSTANT
COLD-SIDE DP-OPTION=CONSTANT

BLOCK B5 HEATX
PARAM T-COLD=870. MIN-TAPP=5. U-OPTION=PHASE &
F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
FEEDS HOT=13 COLD=7
PRODUCTS HOT=H2 COLD=8
HOT-SIDE DP-OPTION=CONSTANT
COLD-SIDE DP-OPTION=CONSTANT

BLOCK B12 HEATX
PARAM T-HOT=130. PRES-COLD=2. U-OPTION=PHASE &
F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
FEEDS HOT=14 COLD=17
PRODUCTS HOT=16 COLD=FEEDH20
HOT-SIDE DP-OPTION=CONSTANT
COLD-SIDE DP-OPTION=CONSTANT

BLOCK B7 RSTOIC
PARAM TEMP=900. PRES=60. HEAT-OF-REAC=NO
STOIC 1 MIXED WATER -1. / OXYGE-01 0.5 / HYDRO-01 1.
CONV 1 MIXED WATER 1.

BLOCK B1 COMPR
PARAM TYPE=ISENTROPIC PRATIO=0.368098 SEFF=0.9 NPHASE=1
BLOCK-OPTION FREE-WATER=NO
EO-CONV-OPTI

STREAM-REPOR MOLEFLOW MASSFLOW
PROPERTY-REP NOPARAM-PLUS
; ; ; ;
*** INPUT TRANSLATOR MESSAGES ***

PDF updated

TIME = 0.29
*** CALCULATION TRACE ***

*** FLOWSHEET ANALYSIS MESSAGES ***

FLOWSHEET CONNECTIVITY BY STREAMS

<table>
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<th>DEST</th>
<th>STREAM</th>
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<tr>
<td>2</td>
<td>B1</td>
<td>B3</td>
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FLOWSHEET CONNECTIVITY BY BLOCKS

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<td>ROUT</td>
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<td>11 13</td>
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<td>B11</td>
<td>O2 H2</td>
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<tr>
<td>B12</td>
<td>14 17</td>
<td>16 FEEDH20</td>
</tr>
<tr>
<td>B1</td>
<td>1</td>
<td>2</td>
</tr>
</tbody>
</table>

BLOCK $SOLVER01 (METHOD: WEGSTEIN) HAS BEEN DEFINED TO CONVERGE
STREAMS: ROUT 9 FEEDH20

COMPUTATION ORDER FOR THE FLOWSHEET IS:
$SOLVER01 B2 REACTOR B1 B3 B9 B7 B8 B4 B5 B11 B12 B6
(RETURN $SOLVER01)

Calculations begin time 0.44
CONVERGENCE BLOCK $OLVER01 METHOD: WEGSTEIN
TIME = 0.46

ENTHALPY CALCULATION FOR INLET STREAM ROUT OF BLOCK B2
TIME = 0.47
KODE = 2 NTRIAL = 0 T = 923.1500 P = 2.000000E+07 V = 1.00000 Q = 0.000000E+00

ENTHALPY CALCULATION FOR INLET STREAM FEEDH20 OF BLOCK B2
TIME = 0.47
KODE = 2 NO. TEMP ITER = 1 TEMP = 303.150 KPHASE = 2 KODE = 2 T = 303.150 P = 100000. Q = 0.000000E+00

UOS BLOCK B2 MODEL: HEATX SPECIFICATION: EXCHANGER DUTY FLOW TYPE: COUNTERCURRENT HOT: TIN= 923.15 PIN=0.20000E+08 COLD: TIN= 303.15 PIN=0.10000E+06
DUTY=0.12960E+09

UOS BLOCK REACTOR MODEL: HEATER
TIME = 0.49
NO. TEMP ITER = 8 TEMP = 296.178 NO. TEMP ITER = 11 TEMP = 923.149
KODE = 1 NTRIAL = 1 T = 923.1491 P = 2.000000E+07 V = 1.00000 Q = 0.000000E+00

UOS BLOCK B1 MODEL: COMPR
TIME = 0.52

* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B1" (MODEL: "COMPR")

FEED STREAM IS BELOW DEW POINT
OUTLET TEMP = 440.2 OUTLET PRES = 0.6000E+07 INDICATED HP = -0.5302E+07 BRAKE HP = -0.5302E+07
ISENTR TEMP = 433.3 CALC ISENTR EFF = 0.9000 ISENTR HP = -0.5891E+07 HP = -0.1471E+08

UOS BLOCK B3 MODEL: FSPLIT
TIME = 0.55
KODE = 1 NO. TEMP ITER = 1 TEMP = 440.176 KPHASE = 1 KODE = 1 T = 440.176 P = 6.000000E+06 Q = 0.000000E+00
SPLIT FRACTIONS: 0.36530D+00 0.63470D+00
UOS BLOCK B9  MODEL: HEATER  TIME = 0.58

* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B9" (MODEL: "HEATER")

(UHE01.4)
ZERO FEED TO THE BLOCK. BLOCK BYPASSED

UOS BLOCK B7  MODEL: RSTOIC  TIME = 0.61

* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B7" (MODEL: "RSTOIC")

(URE07.1)
TOTAL FLOW IS ZERO

UOS BLOCK B8  MODEL: SEP  TIME = 0.66

* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B8" (MODEL: "SEP")

(USP03I.1)
ZERO FEED TO THE BLOCK. BLOCK BYPASSED

UOS BLOCK B4  MODEL: HEATX  TIME = 0.71

* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B4" (MODEL: "HEATX")

(UHE02I.1)
AT LEAST ONE FEED HAS ZERO FLOW
BLOCK BYPASSED

UOS BLOCK B5  MODEL: HEATX  TIME = 0.75

* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B5" (MODEL: "HEATX")

(UHE02I.1)
AT LEAST ONE FEED HAS ZERO FLOW
BLOCK BYPASSED

UOS BLOCK B11  MODEL: MIXER  TIME = 0.80

* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B11"
(MODEL: "MIXER")

(UMX011.1)
ZERO FEED TO BLOCK.
ENTHALPY CALCULATION FOR INLET STREAM 17 OF BLOCK B12
TIME = 0.83
  KODE = 2 NTRIAL = 1 T = 293.1500 P = 100000. V = 0.000000E+00 Q = 0.000000E+00

UOS BLOCK B12 MODEL: HEATX TIME = 0.85

* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B12"
(MODEL: "HEATX")
(UHE021.1)
AT LEAST ONE FEED HAS ZERO FLOW
BLOCK BYPASSED

UOS BLOCK B6 MODEL: MIXER TIME = 0.90
  KODE = 1 NO. TEMP ITER = 12 TEMP = 440.176
  KPHASE = 1 KODE = 1 T = 440.176 P = 6.000000E+06 Q = 0.000000E+00

CONVERGENCE BLOCK $OLVER01 METHOD: WEGSTEIN
TIME = 0.91

--FLASH TEAR STREAM ROUT
NO. TEMP ITER = 1 TEMP = 923.149
  KODE = 1 NTRIAL = 0 T = 923.1491 P = 2.000000E+07 V = 1.00000 Q = 0.000000E+00

--FLASH TEAR STREAM 9
  KODE = 1 NO. TEMP ITER = 1 TEMP = 440.176
  KPHASE = 1 KODE = 1 T = 440.176 P = 6.000000E+06 Q = 0.000000E+00

--FLASH TEAR STREAM FEEDH20
  NO. TEMP ITER = 5 TEMP = 293.150
  KODE = 1 NTRIAL = 2 T = 293.1500 P = 100000. V = 0.000000E+00 Q = 0.000000E+00

LOOP $OLVER01 ITER 1: 3 VARS NOT CONVERGED, MAX ERR/TOL 0.10000E+07 TIME = 0.93

UOS BLOCK B2 MODEL: HEATX TIME = 0.94
  SPECIFICATION: EXCHANGER DUTY 0.12960E+09
  FLOW TYPE: COUNTERCURRENT
  HOT: TIN= 923.15 PIN=0.200000E+08 TOUT= 762.98 POUT=0.200000E+08
  COLD: TIN= 293.15 PIN=0.100000E+06 TOUT= 620.71 POUT=0.163000E+08
  DUTY=0.12960E+09

UOS BLOCK REACTOR MODEL: HEATER TIME =
  0.96
NO. TEMP ITER = 8 TEMP = 296.178
NO. TEMP ITER = 11 TEMP = 923.149
KODE = 1 NTRIAL = 1 T = 923.1491 P = 2.000000E+07 V = 1.00000 Q = 0.000000E+00

UOS BLOCK B1 MODEL: COMPR TIME = 0.99

* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B1" (MODEL: "COMPR")

  (CMSTIN.9)
  FEED STREAM IS BELOW DEW POINT
  OUTLET TEMP = 407.4 OUTLET PRES = 0.6000E+07 INDICATED HP = -0.5291E+07 BRAKE HP = -0.5291E+07
  ISENTR TEMP = 397.5 CALC ISENTR EFF = 0.9000 ISENTR HP = -0.5879E+07 HP = -0.1468E+08

UOS BLOCK B3 MODEL: FSPLIT TIME = 1.04
KODE = 1 NO. TEMP ITER = 7 TEMP = 407.384
KPHASE = 1 KODE = 1 T = 407.384 P = 6.000000E+06 Q = 0.000000E+00
SPLIT FRACTIONS: 0.36530D+00 0.63470D+00

UOS BLOCK B9 MODEL: HEATER TIME = 1.05
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.000000E+06 V = 1.00000 Q = 9.632341E+07

UOS BLOCK B7 MODEL: RSTOIC TIME = 1.07
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.000000E+06 V = 1.00000 Q = 6.923856E+08

UOS BLOCK B8 MODEL: SEP TIME = 1.10
---FLASH OUTLET STREAM 11 :
  KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.000000E+06 V = 1.00000 Q = 0.000000E+00
  TIME = 1.11
  DUTY = 0.34706E+08
---FLASH OUTLET STREAM 13 :
  KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.000000E+06 V = 1.00000 Q = 0.000000E+00

UOS BLOCK B4 MODEL: HEATX SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 1173.15 PIN= 0.600000E+07 TOUT= 434.64 POUT= 0.600000E+07
COLD: TIN= 407.38 PIN= 0.600000E+07 TOUT= 1143.15 POUT= 0.600000E+07
DUTY = 0.34706E+08

UOS BLOCK B5 MODEL: HEATX SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 1173.15 PIN=0.60000E+07 TOUT= 444.47 POUT=0.60000E+07
COLD: TIN= 407.38 PIN=0.60000E+07 TOUT= 1143.15 POUT=0.60000E+07
DUTY=0.60301E+08

UOS BLOCK B11  MODEL: MIXER  TIME = 1.16
KODE = 1  NO. TEMP ITER =  5  TEMP = 439.955
KPHASE = 1  KODE = 1  T = 439.955  P = 6.000000E+06  Q = 0.000000E+00

UOS BLOCK B12  MODEL: HEATX  TIME = 1.18
SPECIFICATION: HOT OUTLET TEMP 403.15
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 439.96 PIN=0.60000E+07 TOUT= 403.15 POUT=0.60000E+07
COLD: TIN= 293.15 PIN=0.10000E+06 TOUT= 312.26 POUT=0.20000E+06
DUTY=0.46053E+07

UOS BLOCK B6  MODEL: MIXER  TIME = 1.21
KODE = 1  NO. TEMP ITER =  7  TEMP = 1143.15
KPHASE = 1  KODE = 1  T = 1143.15  P = 6.000000E+06  Q = 0.000000E+00

CONVERGENCE BLOCK $OLVER01  METHOD: WEGSTEIN  TIME = 1.22

--FLASH TEAR STREAM ROUT
NO. TEMP ITER =  1  TEMP = 923.149
KODE = 1  NTRIAL =  0  T = 923.1491  P = 2.000000E+07  V = 1.00000  Q = 0.000000E+00

--FLASH TEAR STREAM 9
KODE = 1  NO. TEMP ITER =  7  TEMP = 1143.15
KPHASE = 1  KODE = 1  T = 1143.15  P = 6.000000E+06  Q = 0.000000E+00

--FLASH TEAR STREAM FEEDH20
NO. TEMP ITER =  5  TEMP = 312.256
KODE = 1  NTRIAL =  2  T = 312.2564  P = 200000.  V = 0.000000E+00  Q = 0.000000E+00

LOOP $OLVER01 ITER  2:  3 VARS NOT CONVERGED, MAX ERR/TOL 10000.  TIME = 1.24

UOS BLOCK B2  MODEL: HEATX  TIME = 1.25
SPECIFICATION: EXCHANGER DUTY 0.12960E+09
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 923.15 PIN=0.20000E+08 TOUT= 762.98 POUT=0.20000E+08
COLD: TIN= 312.26 PIN=0.20000E+06 TOUT= 620.71 POUT=0.16300E+08
DUTY=0.12960E+09
UOS BLOCK REACTOR MODEL: HEATER
TIME = 1.27
NO. TEMP ITER = 8 TEMP = 296.178
NO. TEMP ITER = 11 TEMP = 923.149
KODE = 1 NTRIAL = 1 T = 923.1491 P = 2.000000E+07 V = 1.00000 Q = 0.000000E+00

UOS BLOCK B1 MODEL: COMPR
TIME = 1.29

* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B1" (MODEL: "COMPR")

(CMSTIN.9)
FEED STREAM IS BELOW DEW POINT
OUTLET TEMP = 458.8 OUTLET PRES = 0.6000E+07 INDICATED HP = -0.5135E+07 BRAKE HP = -0.5135E+07
ISENTR TEMP = 455.7 CALC ISENTR EFF = 0.9000 ISENTR HP = -0.5705E+07 HP = -0.1425E+08

UOS BLOCK B3 MODEL: FSPLIT
TIME = 1.33
KODE = 1 NO. TEMP ITER = 9 TEMP = 458.810
KPHASE = 1 KODE = 1 T = 458.810 P = 6.0000000E+06 Q = 0.0000000E+00
SPLIT FRACTIONS: 0.36530D+00 0.63470D+00

UOS BLOCK B9 MODEL: HEATER
TIME = 1.35
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.0000000E+06 V = 1.00000 Q = 3.713824E+06

UOS BLOCK B7 MODEL: RSTOIC
TIME = 1.38
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.0000000E+06 V = 1.00000 Q = 6.923856E+08

UOS BLOCK B8 MODEL: SEP
TIME = 1.40
---FLASH OUTLET STREAM 11 :
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.0000000E+06 V = 1.00000 Q = 0.0000000E+00
---FLASH OUTLET STREAM 13 :
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.0000000E+06 V = 1.00000 Q = 0.0000000E+00

UOS BLOCK B4 MODEL: HEATX
TIME = 1.43
SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN = 1173.15 PIN = 0.600000E+07 TOUT = 473.85 POUT = 0.600000E+07
COLD: TIN = 458.81 PIN = 0.600000E+07 TOUT = 1143.15 POUT = 0.600000E+07
DUTY = 0.32967E+08
UOS BLOCK B5  MODEL: HEATX  TIME =  1.44
SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 1173.15 PIN=0.60000E+07 TOUT= 481.50 POUT=0.60000E+07
COLD: TIN= 458.81 PIN=0.60000E+07 TOUT= 1143.15 POUT=0.60000E+07
DUTY=0.57279E+08

UOS BLOCK B11  MODEL: MIXER  TIME =  1.47
KODE = 1  NO. TEMP ITER =  4  TEMP = 477.927
KPHASE =  1 KODE =  1 T = 477.927  P = 6.000000E+06 Q = 0.000000E+00

UOS BLOCK B12  MODEL: HEATX  TIME =  1.49
SPECIFICATION: HOT OUTLET TEMP 403.15
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 477.93 PIN=0.60000E+07 TOUT= 403.15 POUT=0.60000E+07
COLD: TIN= 293.15 PIN=0.10000E+06 TOUT= 332.05 POUT=0.20000E+06
DUTY=0.93666E+07

UOS BLOCK B6  MODEL: MIXER  TIME =  1.50
KODE = 1  NO. TEMP ITER =  1  TEMP = 1143.15
KPHASE =  1 KODE =  1 T = 1143.15  P = 6.000000E+06 Q = 0.000000E+00

CONVERGENCE BLOCK $OLVER01 METHOD: WEGSTEIN
TIME =  1.54

--FLASH TEAR STREAM ROUT
NO. TEMP ITER =  1  TEMP = 923.149
KODE = 1  NTRIAL =  0  T = 923.1491  P = 2.000000E+07  V = 1.00000  Q = 0.000000E+00

--FLASH TEAR STREAM 9
KODE = 1  NO. TEMP ITER =  1  TEMP = 1143.15
KPHASE =  1 KODE =  1 T = 1143.15  P = 6.000000E+06 Q = 0.000000E+00

--FLASH TEAR STREAM FEEDH20
NO. TEMP ITER =  5  TEMP = 332.050
KODE = 1  NTRIAL =  2  T = 332.0498  P = 200000.  V = 0.000000E+00  Q = 0.000000E+00

LOOP $OLVER01 ITER  3:  1 VARS NOT CONVERGED, MAX ERR/TOL
59.642  TIME =  1.55

UOS BLOCK B2  MODEL: HEATX  TIME =  1.55
SPECIFICATION: EXCHANGER DUTY 0.12960E+09
FLOW TYPE: COUNTERCURRENT

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HOT: TIN= 923.15 PIN=0.20000E+08 TOUT= 762.98 POUT=0.20000E+08
COLD: TIN= 332.05 PIN=0.20000E+06 TOUT= 620.71 POUT=0.16300E+08
DUTY=0.12960E+09

UOS BLOCK REACTOR MODEL: HEATER TIME =
1.58
NO. TEMP ITER = 8 TEMP = 296.178
NO. TEMP ITER = 11 TEMP = 923.149
KODE = 1 NTRIAL = 1 T = 923.1491 P = 2.000000E+07 V = 1.00000 Q = 0.000000E+00

UOS BLOCK B1 MODEL: COMPR TIME =
1.60
* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B1" (MODEL: "COMPR")
(CMSTIN.9)
FEED STREAM IS BELOW DEW POINT
OUTLET TEMP = 465.2 OUTLET PRES = 0.60000E+07 INDICATED HP = -0.5975E+07 BRAKE HP = -0.5975E+07
ISENTR TEMP = 463.8 CALC ISENTR EFF = 0.9000 ISENTR HP = -0.6639E+07 HP = -0.1658E+08

UOS BLOCK B3 MODEL: FSPLIT TIME =
1.64
KODE = 1 NO. TEMP ITER = 7 TEMP = 465.175
KPHASE = 1 KODE = 1 T = 465.175 P = 6.000000E+06 Q = 0.000000E+00
SPLIT FRACTIONS: 0.36530D+00 0.63470D+00

UOS BLOCK B9 MODEL: HEATER TIME =
1.68
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.000000E+06 V = 1.00000 Q = 3.713824E+06

UOS BLOCK B7 MODEL: RSTOIC TIME =
1.69
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.000000E+06 V = 1.00000 Q = 6.923856E+08

UOS BLOCK B8 MODEL: SEP TIME =
1.71
---FLASH OUTLET STREAM 11
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.000000E+06 V = 1.00000 Q = 0.000000E+00
---FLASH OUTLET STREAM 13
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.000000E+06 V = 1.00000 Q = 0.000000E+00

UOS BLOCK B4 MODEL: HEATX TIME =
1.74
SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT
UOS BLOCK B5  MODEL: HEATX  TIME =  1.75
SPECIFICATION: COLD OUTLET TEMP  1143.2
FLOW TYPE:  COUNTERCURRENT
HOT: TIN=  1173.15 PIN=0.60000E+07 TOUT=  511.99 POUT=0.60000E+07
COLD: TIN=  465.17 PIN=0.60000E+07 TOUT=  1143.15 POUT=0.60000E+07
DUTY=0.54791E+08

UOS BLOCK B11  MODEL: MIXER  TIME =  1.79
KODE = 1  NO. TEMP ITER =  4  TEMP =  509.133
KPHASE =  1  KODE =  1  T   =  509.133  P  =  6.000000E+06  Q =  0.000000E+00

UOS BLOCK B12  MODEL: HEATX  TIME =  1.80
SPECIFICATION: HOT OUTLET TEMP  403.15
FLOW TYPE:  COUNTERCURRENT
HOT: TIN=  509.13 PIN=0.60000E+07 TOUT=  403.15 POUT=0.60000E+07
COLD: TIN=  293.15 PIN=0.10000E+06 TOUT=  348.32 POUT=0.20000E+06
DUTY=0.13288E+08

UOS BLOCK B6  MODEL: MIXER  TIME =  1.83
KODE = 1  NO. TEMP ITER =  1  TEMP =  1143.15
KPHASE =  1  KODE =  1  T   =  1143.15  P  =  6.000000E+06  Q =  0.000000E+00

CONVERGENCE BLOCK $OLVER01 METHOD: WEGSTEIN  TIME =  1.85

--FLASH TEAR STREAM ROUT
NO. TEMP ITER =  1  TEMP =  923.149
KODE = 1  NTRIAL =  0  T   =  923.1491  P  =  2.000000E+07  V =  1.00000  Q =  0.000000E+00

--FLASH TEAR STREAM 9
KODE = 1  NO. TEMP ITER =  1  TEMP =  1143.15
KPHASE =  1  KODE =  1  T   =  1143.15  P  =  6.000000E+06  Q =  0.000000E+00

--FLASH TEAR STREAM FEEDH2O
KODE = 1  NTRIAL =  3  T   =  395.2141  P  =  200000.  V =  5.951367E-02  Q =  0.000000E+00

LOOP $OLVER01 ITER  4:  1 VARS NOT CONVERGED, MAX ERR/TOL
49.415  TIME =  1.86

UOS BLOCK B2  MODEL: HEATX  TIME =  1.88
SPECIFICATION: EXCHANGER DUTY  0.12960E+09
FLOW TYPE:  COUNTERCURRENT
HOT:  TIN= 923.15 PIN=0.20000E+08 TOUT= 762.98 POUT=0.20000E+08
COLD: TIN= 395.21 PIN=0.20000E+06 TOUT= 724.80 POUT=0.16300E+08
DUTY=0.12960E+09

UOS BLOCK REACTOR MODEL: HEATER
TIME =
1.89
NO. TEMP ITER =  8  TEMP = 296.178
NO. TEMP ITER = 11    TEMP = 923.149
KODE = 1  NTRIAL =  1  T = 923.1491  P = 2.000000E+07  V = 1.00000  Q =
0.000000E+00

UOS BLOCK B1 MODEL: COMPR
TIME = 1.93
OUTLET TEMP =  566.4  OUTLET PRES = 0.6000E+07  INDICATED HP =
0.1081E+08  BRAKE HP = -0.1081E+08
ISENTR TEMP =  557.3  CALC ISENTR EFF = 0.9000  ISENTR HP =
0.1202E+08  HP = -0.3002E+08

UOS BLOCK B3 MODEL: FSPLIT
TIME = 1.94
KODE = 1  NO. TEMP ITER =  6  TEMP = 566.390
KPHASE = 1  KODE = 1  T = 566.390  P = 6.000000E+06  Q = 0.000000E+00
SPLIT FRACTIONS: 0.36530D+00  0.63470D+00

UOS BLOCK B9 MODEL: HEATER
TIME = 1.97
KODE = 2  NTRIAL =  0  T=1173.1500  P = 6.000000E+06  V = 1.00000  Q =
3.713824E+06

UOS BLOCK B7 MODEL: RSTOIC
TIME = 1.99
KODE = 2  NTRIAL =  0  T=1173.1500  P = 6.000000E+06  V = 1.00000  Q =
6.923856E+08

UOS BLOCK B8 MODEL: SEP
TIME = 2.00
---FLASH OUTLET STREAM 11
KODE = 2  NTRIAL =  0  T=1173.1500  P = 6.000000E+06  V = 1.00000  Q =
0.000000E+00
---FLASH OUTLET STREAM 13
KODE = 2  NTRIAL =  0  T=1173.1500  P = 6.000000E+06  V = 1.00000  Q =
0.000000E+00

UOS BLOCK B4 MODEL: HEATX
SPECIFICATION: COLD OUTLET TEMP  1143.2
FLOW TYPE:  COUNTERCURRENT
HOT:  TIN= 1173.15 PIN=0.60000E+07 TOUT= 646.51 POUT=0.60000E+07
COLD: TIN= 566.39 PIN=0.60000E+07 TOUT= 1143.15 POUT=0.60000E+07
DUTY=0.25183E+08

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UOS BLOCK B5  MODEL: HEATX  
SPECIFICATION: COLD OUTLET TEMP  1143.2  
FLOW TYPE:  COUNTERCURRENT  
HOT:  TIN= 1173.15  PIN=0.60000E+07  TOUT= 647.33  POUT=0.60000E+07  
COLD:  TIN= 566.39  PIN=0.60000E+07  TOUT= 1143.15  POUT=0.60000E+07  
DUTY=0.43755E+08 

UOS BLOCK B11  MODEL: MIXER  
KODE = 1  NO. TEMP ITER = 4  TEMP = 646.656  
KPHASE = 1  KODE = 1  T = 646.656  P = 6.000000E+06  Q = 0.000000E+00 

UOS BLOCK B12  MODEL: HEATX  
SPECIFICATION: HOT OUTLET TEMP  403.15  
FLOW TYPE:  COUNTERCURRENT  
HOT:  TIN= 646.66  PIN=0.60000E+07  TOUT= 403.15  POUT=0.60000E+07  
COLD:  TIN= 293.15  PIN=0.10000E+06  TOUT= 395.21  POUT=0.20000E+06  
DUTY=0.30675E+08 

UOS BLOCK B6  MODEL: MIXER  
KODE = 1  NO. TEMP ITER = 1  TEMP = 1143.15  
KPHASE = 1  KODE = 1  T = 1143.15  P = 6.000000E+06  Q = 0.000000E+00 

CONVERGENCE BLOCK SOLVER01  METHOD: WEGSTEIN  
TIME = 2.14 

--FLASH TEAR STREAM ROUT  
NO. TEMP ITER = 1  TEMP = 923.149  
KODE = 1  NTRIAL = 0  T = 923.1491  P = 2.000000E+07  V = 1.00000  Q = 0.000000E+00 

--FLASH TEAR STREAM 9  
KODE = 1  NO. TEMP ITER = 1  TEMP = 1143.15  
KPHASE = 1  KODE = 1  T = 1143.15  P = 6.000000E+06  Q = 0.000000E+00 

--FLASH TEAR STREAM FEEDH20  
KODE = 1  NTRIAL = 1  T = 395.2146  P = 200000  V = 2.309195E-02  Q = 0.000000E+00 

LOOP SOLVER01 ITER 5: 1 VARS NOT CONVERGED, MAX ERR/TOL - 11.910  TIME = 2.16 

UOS BLOCK B2  MODEL: HEATX  
SPECIFICATION: EXCHANGER DUTY  0.12960E+09  
FLOW TYPE:  COUNTERCURRENT  
HOT:  TIN= 923.15  PIN=0.20000E+08  TOUT= 762.98  POUT=0.20000E+08
COLD: TIN= 395.21 PIN=0.20000E+06 TOUT= 697.99 POUT=0.16300E+08
DUTY=0.12960E+09

UOS BLOCK REACTOR MODEL: HEATER

TIME = 2.19
NO. TEMP ITER = 8 TEMP = 296.178
NO. TEMP ITER = 11 TEMP = 923.149
KODE = 1 NTRIAL = 1 T = 923.1491 P = 2.0000000E+07 V = 1.00000 Q = 0.0000000E+00

UOS BLOCK B1 MODEL: COMPR
TIME = 2.22
OUTLET TEMP = 541.5 OUTLET PRES = 0.6000E+07 INDICATED HP = -0.9929E+07 BRAKE HP = -0.9929E+07
ISENTR TEMP = 533.6 CALC ISENTR EFF = 0.9000 ISENTR HP = -0.1103E+08 HP = -0.2756E+08

UOS BLOCK B3 MODEL: FSPLIT
TIME = 2.24
KODE = 1 NO. TEMP ITER = 5 TEMP = 541.525
KPHASE = 1 KODE = 1 T = 541.525 P = 6.000000E+06 Q = 0.0000000E+00
SPLIT FRACTIONS: 0.36530D+00 0.63470D+00

UOS BLOCK B9 MODEL: HEATER
TIME = 2.27
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.000000E+06 V = 1.00000 Q = 3.713824E+06

UOS BLOCK B7 MODEL: RSTOIC
TIME = 2.29
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.000000E+06 V = 1.00000 Q = 6.923856E+08

UOS BLOCK B8 MODEL: SEP
TIME = 2.30
---FLASH OUTLET STREAM 11 :
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.000000E+06 V = 1.00000 Q = 0.0000000E+00
---FLASH OUTLET STREAM 13 :
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.000000E+06 V = 1.00000 Q = 0.0000000E+00

UOS BLOCK B4 MODEL: HEATX
SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 1173.15 PIN=0.60000E+07 TOUT= 619.87 POUT=0.60000E+07
COLD: TIN= 541.53 PIN=0.60000E+07 TOUT= 1143.15 POUT=0.60000E+07
DUTY=0.26400E+08

UOS BLOCK B5 MODEL: HEATX
SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 1173.15 PIN=0.60000E+07 TOUT= 621.38 POUT=0.60000E+07
COLD: TIN= 541.53 PIN=0.60000E+07 TOUT= 1143.15 POUT=0.60000E+07
DUTY=0.45870E+08

UOS BLOCK B11 MODEL: MIXER TIME = 2.38
KODE = 1 NO. TEMP ITER = 4 TEMP = 620.412
KPHASE = 1 KODE = 1 T = 620.412 P = 6.000000E+06 Q = 0.000000E+00

UOS BLOCK B12 MODEL: HEATX TIME = 2.39
SPECIFICATION: HOT OUTLET TEMP 403.15
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 620.41 PIN=0.60000E+07 TOUT= 403.15 POUT=0.60000E+07
COLD: TIN= 293.15 PIN=0.10000E+06 TOUT= 395.21 POUT=0.20000E+06
DUTY=0.27342E+08

UOS BLOCK B6 MODEL: MIXER TIME = 2.43
KODE = 1 NO. TEMP ITER = 1 TEMP = 1143.15
KPHASE = 1 KODE = 1 T = 1143.15 P = 6.000000E+06 Q = 0.000000E+00

CONVERGENCE BLOCK $OLVER01 METHOD: WEGSTEIN
TIME = 2.46

LOOP $OLVER01 ITER 6: *** CONVERGED ***, MAX ERR/TOL -0.42294
TIME = 2.47

GENERATING RESULTS FOR UOS BLOCK B2 MODEL: HEATX
TIME = 2.47
SPECIFICATION: EXCHANGER DUTY 0.12960E+09
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 923.15 PIN=0.20000E+08 TOUT= 762.98 POUT=0.20000E+08
COLD: TIN= 395.21 PIN=0.20000E+06 TOUT= 697.99 POUT=0.16300E+08
AREA= 476.88 DUTY=0.12960E+09 FT=1.00000

GENERATING RESULTS FOR UOS BLOCK B4 MODEL: HEATX
TIME = 2.50
SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 1173.15 PIN=0.60000E+07 TOUT= 619.87 POUT=0.60000E+07
COLD: TIN= 541.53 PIN=0.60000E+07 TOUT= 1143.15 POUT=0.60000E+07
AREA= 616.70 DUTY=0.26400E+08 FT=1.00000

GENERATING RESULTS FOR UOS BLOCK B5 MODEL: HEATX
TIME = 2.52
SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 1173.15 PIN=0.60000E+07 TOUT= 621.38 POUT=0.60000E+07
COLD: TIN= 541.53 PIN=0.60000E+07 TOUT=1143.15 POUT=0.60000E+07
AREA= 1059.7 DUTY=0.45870E+08 FT=1.00000

GENERATING RESULTS FOR UOS BLOCK B12  MODEL: HEATX
TIME =  2.54
SPECIFICATION: HOT OUTLET TEMP  403.15
FLOW TYPE:  COUNTERCURRENT
HOT: TIN= 620.41 PIN=0.60000E+07 TOUT= 403.15 POUT=0.60000E+07
COLD: TIN= 293.15 PIN=0.10000E+06 TOUT= 395.21 POUT=0.20000E+06
AREA= 205.18 DUTY=0.27342E+08 FT=1.00000

Report Writer entered
Results generated
RUN SAVED

*** SUMMARY OF ERRORS ***

   PHYSICAL
   PROPERTY  SYSTEM  SIMULATION
TERMINAL ERRORS 0 0 0
SEVERE ERRORS 0 0 0
ERRORS 0 0 0
WARNINGS 0 0 11
*** CALCULATION TRACE ***

RUN SAVED

NO ERRORS OR WARNINGS GENERATED

RUN SAVED

NO ERRORS OR WARNINGS GENERATED
*** INPUT SPECIFICATION MESSAGES ***

;Directory H:\ Runid HTSE FINAL H2 ONLY 650C
;

STREAM 17
  SUBSTREAM MIXED TEMP=20. PRES=1. MASS-FLOW=93. <kg/sec>
    MASS-FRAC WATER 1.

STREAM FEEDH20
  SUBSTREAM MIXED TEMP=30. PRES=1. MASS-FLOW=93. <kg/sec> &
    FREE-WATER=NO NPHASE=1 PHASE=L
    MASS-FRAC WATER 1.

STREAM RIN
  SUBSTREAM MIXED TEMP=489.2817 PRES=200. &
    MASS-FLOW=1143.152 <kg/sec>
    MASS-FRAC CARBO-01 1.

STREAM ROUT
  SUBSTREAM MIXED TEMP=650. PRES=200. &
    MASS-FLOW=1143.152 <kg/sec>
    MASS-FRAC CARBO-01 1.

CHANGES WERE MADE TO BLOCK REACTOR 07/26/2006 10:31:18:99
BLOCK REACTOR HEATER
  PARAM PRES=200. DUTY=234.6 <MW>

BLOCK B2 HEATX
  PARAM DUTY=234.6 <MW> PRES-COLD=163. U-OPTION=PHASE &
    F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
    FEEDS HOT=ROUT COLD=FEEDH20
    PRODUCTS HOT=RIN COLD=1
    HOT-SIDE DP-OPTION=CONSTANT
    COLD-SIDE DP-OPTION=CONSTANT

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Calculations begin

SIMULATION CALCULATIONS BEGIN

CONVERGENCE BLOCK $OLVER01 METHOD: WEGSTEIN
TIME = 337.24

ENTHALPY CALCULATION FOR INLET STREAM ROUT OF BLOCK B2
TIME = 337.28
KODE = 2 NTRIAL = 0 T = 923.1500 P = 2.000000E+07 V = 1.000000 Q =
0.000000E+00

ENTHALPY CALCULATION FOR INLET STREAM FEEDH20 OF BLOCK B2
TIME = 337.39
KODE = 2 NO. TEMP ITER = 1 TEMP = 303.150 KPHASE = 2 KODE = 2 T =
303.150 P = 100000. Q = 0.000000E+00

UOS BLOCK B2 MODEL: HEATX
TIME = 337.41
SPECIFICATION: EXCHANGER DUTY 0.23460E+09
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 923.15 PIN=0.20000E+08 TOUT= 759.46 POUT=0.20000E+08
COLD: TIN= 303.15 PIN=0.10000E+06 TOUT= 620.71 POUT=0.16300E+08
DUTY=0.23460E+09

UOS BLOCK REACTOR MODEL: HEATER
TIME = 337.59
NO. TEMP ITER = 8 TEMP = 296.178
NO. TEMP ITER = 11 TEMP = 923.149
KODE = 1 NTRIAL = 1 T = 923.1491 P = 2.000000E+07 V = 1.000000 Q =
0.000000E+00

UOS BLOCK B1 MODEL: COMPR
TIME = 337.61

* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B1" (MODEL:
"COMPR")

(CMSTIN.9)
FEED STREAM IS BELOW DEW POINT
OUTLET TEMP = 393.8   OUTLET PRES = 0.6000E+07   INDICATED HP = -0.9351E+07   BRAKE HP = -0.9351E+07
ISENTR TEMP = 383.7   CALC ISENTR EFF = 0.9000   ISENTR HP = -0.1039E+08   HP = -0.4827E+08

UOS BLOCK B3   MODEL: FSPLIT   TIME = 337.64
KODE = 1   NO. TEMP ITER = 6   TEMP = 393.850
KPHASE = 1   KODE = 1   T = 393.850   P = 6.000000E+06   Q = 0.000000E+00
SPLIT FRACTIONS: 0.36530D+00   0.63470D+00

UOS BLOCK B9   MODEL: HEATER   TIME = 337.64
KODE = 2   NTRIAL = 0   T = 1173.1500   P = 6.000000E+06   V = 1.00000   Q = 3.713824E+06

UOS BLOCK B7   MODEL: RSTOIC   TIME = 337.64
KODE = 2   NTRIAL = 0   T = 1173.1500   P = 6.000000E+06   V = 1.00000   Q = 6.923856E+08

UOS BLOCK B8   MODEL: SEP   TIME = 337.66
---FLASH OUTLET STREAM 11:
KODE = 2   NTRIAL = 0   T = 1173.1500   P = 6.000000E+06   V = 1.00000   Q = 0.000000E+00
---FLASH OUTLET STREAM 13:
KODE = 2   NTRIAL = 0   T = 1173.1500   P = 6.000000E+06   V = 1.00000   Q = 0.000000E+00

UOS BLOCK B4   MODEL: HEATX   TIME = 337.66
SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT

** ERROR WHILE EXECUTING UNIT OPERATIONS BLOCK: "B4" (MODEL: "HEATX")
(HEATX.4)
TEMPERATURE CROSSOVER DETECTED
RE-CALCULATING WITH MINIMUM APPROACH TEMP. SPEC
HOT: TIN= 1173.15   PIN=0.600000E+07   TOUT= 394.85   POUT=0.600000E+07
COLD: TIN= 393.85   PIN=0.600000E+07   TOUT= 790.28   POUT=0.600000E+07
DUTY=0.36469E+08

UOS BLOCK B5   MODEL: HEATX   TIME = 337.67
SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT
** ERROR WHILE EXECUTING UNIT OPERATIONS BLOCK: "B5" (MODEL: "HEATX")

(HEATX.4)
TEMPERATURE CROSSOVER DETECTED
RE-CALCULATING WITH MINIMUM APPROACH TEMP. SPEC
HOT: TIN= 1173.15 PIN=0.60000E+07 TOUT= 398.85 POUT=0.60000E+07
COLD: TIN= 393.85 PIN=0.60000E+07 TOUT= 795.08 POUT=0.60000E+07
DUTY=0.64024E+08

UOS BLOCK B11 MODEL: MIXER

TIME =
337.67
KODE = 1 NO. TEMP ITER = 5 TEMP = 396.112
KPHASE = 1 KODE = 1 T = 396.112 P = 6.000000E+06 Q = 0.000000E+00

ENTHALPY CALCULATION FOR INLET STREAM 17 OF BLOCK B12

TIME = 337.67
KODE = 2 NTRIAL = 1 T = 293.1500 P = 100000. V = 0.000000E+00 Q = 0.000000E+00

UOS BLOCK B12 MODEL: HEATX

TIME =
337.69

** ERROR WHILE EXECUTING UNIT OPERATIONS BLOCK: "B12" (MODEL: "HEATX")

(HXZCSP.1)
INVALID HOT STREAM TEMPERATURE SPECIFICATION
T-SPEC = 4.0315000D+02 IS MORE THAN THIN = 3.9611205D+02

UOS BLOCK B6 MODEL: MIXER

TIME = 337.69
KODE = 1 NO. TEMP ITER = 7 TEMP = 793.329
KPHASE = 1 KODE = 1 T = 793.329 P = 6.000000E+06 Q = 0.000000E+00

CONVERGENCE BLOCK $OLVER01 METHOD: WEGSTEIN

TIME = 337.69

--FLASH TEAR STREAM ROUT
NO. TEMP ITER = 1 TEMP = 923.149
KODE = 1 NTRIAL = 0 T = 923.1491 P = 2.000000E+07 V = 1.00000 Q = 0.000000E+00

--FLASH TEAR STREAM 9
KODE = 1 NO. TEMP ITER = 7 TEMP = 793.329
KPHASE = 1 KODE = 1 T = 793.329 P = 6.000000E+06 Q = 0.000000E+00

--FLASH TEAR STREAM FEEDH2O
NO. TEMP ITER = 5  TEMP = 257.436
KODE = 1 NTRIAL = 2  T = 257.4357  P = 100000  V = 0.000000E+00  Q =
0.000000E+00

LOOP $SOLVER01  ITER  1:  4 VARS NOT CONVERGED, MAX ERR/TOL
8600.0   TIME =   337.74

UOS BLOCK B2  MODEL: HEATX   TIME =
337.74
SPECIFICATION: EXCHANGER DUTY  0.23460E+09
FLOW TYPE: COUNTERCURRENT
HOT: TIN=  923.15  PIN=0.20000E+08  TOUT= 759.46  POUT=0.20000E+08
COLD: TIN= 257.44  PIN=0.10000E+06  TOUT= 620.71  POUT=0.16300E+08
    DUTY=0.23460E+09

UOS BLOCK REACTOR   MODEL: HEATER   TIME =
337.74
NO. TEMP ITER = 8  TEMP = 296.178
NO. TEMP ITER = 11  TEMP = 923.149
KODE = 1 NTRIAL = 1  T = 923.1491  P = 2.000000E+07  V = 1.00000  Q =
0.000000E+00

UOS BLOCK B1   MODEL: COMPR   TIME =
337.74

* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B1" (MODEL:
"COMPR")

   (CMSTIN.9)
FEED STREAM IS BELOW DEW POINT
OUTLET TEMP = 266.9  OUTLET PRES = 0.6000E+07  INDICATED HP = -
0.1330E+06  BRAKE HP = -0.1330E+06
ISENTR TEMP = 266.8  CALC ISENTR EFF = 0.9000  ISENTR HP = -
0.1478E+06  HP = -0.6865E+06

UOS BLOCK B3   MODEL: FSPLIT   TIME = 337.74
KODE = 1 NO. TEMP ITER = 6  TEMP = 266.927
KPHASE = 1 KODE = 1  T = 266.927  P = 6.000000E+06  Q = 0.000000E+00
SPLIT FRACTIONS: 0.36530D+00  0.63470D+00

UOS BLOCK B9   MODEL: HEATER   TIME =
337.74
KODE = 2 NTRIAL = 0  T =1173.1500  P = 6.000000E+06  V = 1.00000  Q =
8.461461E+07

UOS BLOCK B7   MODEL: RSTOIC   TIME = 337.74
KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 1.287837E+09

UOS BLOCK B8  MODEL: SEP  TIME = 337.74
---FLASH OUTLET STREAM 11 :
   KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 0.000000E+00
   ---FLASH OUTLET STREAM 13 :
      KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 0.000000E+00

UOS BLOCK B4  MODEL: HEATX  TIME = 337.74
SPECIFICATION: COLD OUTLET TEMP  1143.2
FLOW TYPE:  COUNTERCURRENT
HOT:  TIN= 1173.15  PIN=0.600000E+07  TOUT= 377.72  POUT=0.600000E+07
COLD:  TIN= 266.93  PIN=0.600000E+07  TOUT= 1143.15  POUT=0.600000E+07
   DUTY=0.69246E+08

UOS BLOCK B5  MODEL: HEATX  TIME = 337.74
SPECIFICATION: COLD OUTLET TEMP  1143.2
FLOW TYPE:  COUNTERCURRENT
HOT:  TIN= 1173.15  PIN=0.600000E+07  TOUT= 390.75  POUT=0.600000E+07
COLD:  TIN= 266.93  PIN=0.600000E+07  TOUT= 1143.15  POUT=0.600000E+07
   DUTY=0.12031E+09

UOS BLOCK B11  MODEL: MIXER  TIME = 337.74
   KODE = 1  NO. TEMP ITER = 4  TEMP = 384.740
   KPHASE = 1  KODE = 1  T = 384.740  P = 6.000000E+06  Q = 0.000000E+00

UOS BLOCK B12  MODEL: HEATX  TIME = 337.74

** ERROR WHILE EXECUTING UNIT OPERATIONS BLOCK: "B12" (MODEL: "HEATX")

   (HXZCSP.1)
   INVALID HOT STREAM TEMPERATURE SPECIFICATION
   T-SPEC = 4.0315000D+02 IS MORE THAN THIN = 3.8473980D+02

UOS BLOCK B6  MODEL: MIXER  TIME = 337.74
   KODE = 1  NO. TEMP ITER = 6  TEMP = 1143.15
   KPHASE = 1  KODE = 1  T = 1143.15  P = 6.000000E+06  Q = 0.000000E+00

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CONVERGENCE BLOCK $SOLVER01$ METHOD: WEGSTEIN
TIME = 337.74

--FLASH TEAR STREAM ROUT
NO. TEMP ITER = 1 TEMP = 923.149
KODE = 1 NTRIAL = 0 T = 923.1491 P = 2.000000E+07 V = 1.00000 Q =
0.000000E+00

--FLASH TEAR STREAM 9
KODE = 1 NO. TEMP ITER = 6 TEMP = 1143.15
KPHASE = 1 KODE = 1 T = 1143.15 P = 6.000000E+06 Q = 0.000000E+00

--FLASH TEAR STREAM FEEDH2O
NO. TEMP ITER = 5 TEMP = 293.150
KODE = 1 NTRIAL = 2 T = 293.1500 P = 100000. V = 0.000000E+00 Q =
0.000000E+00

LOOP $SOLVER01$ ITER 2: 2 VARS NOT CONVERGED, MAX ERR/TOL
668.04 TIME = 337.74

UOS BLOCK B2 MODEL: HEATX TIME =
337.74
SPECIFICATION: EXCHANGER DUTY 0.23460E+09
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 923.15 PIN=0.20000E+08 TOUT= 759.46 POUT=0.20000E+08
COLD: TIN= 293.15 PIN=0.10000E+06 TOUT= 620.71 POUT=0.16300E+08
DUTY=0.23460E+09

UOS BLOCK REACTOR MODEL: HEATER TIME =
337.74
NO. TEMP ITER = 8 TEMP = 296.178
NO. TEMP ITER = 11 TEMP = 923.149
KODE = 1 NTRIAL = 1 T = 923.1491 P = 2.000000E+07 V = 1.00000 Q =
0.000000E+00

UOS BLOCK B1 MODEL: COMPR TIME =
337.74

* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B1" (MODEL:
"COMPR")
(CMSTIN.9)
FEED STREAM IS BELOW DEW POINT
OUTLET TEMP = 380.8 OUTLET PRES = 0.6000E+07 INDICATED HP = -
0.6203E+07 BRAKE HP = -0.6203E+07
ISENTR TEMP = 373.7 CALC ISENTR EFF = 0.9000 ISENTR HP = -
0.6893E+07 HP = -0.3202E+08
UOS BLOCK B3  MODEL: FSPLIT  TIME =  337.74
KODE = 1  NO. TEMP ITER =  6  TEMP = 380.783
KPHASE =  1 KODE = 1 T = 380.783  P = 6.000000E+06 Q = 0.000000E+00
SPLIT FRACTIONS: 0.36530D+00  0.63470D+00

UOS BLOCK B9  MODEL: HEATER  TIME = 337.74
KODE = 2  NTRIAL = 0  T =1173.1500  P = 6.000000E+06  V = 1.00000  Q = 6.907713E+06

UOS BLOCK B7  MODEL: RSTOIC  TIME = 337.78
KODE = 2  NTRIAL = 0  T =1173.1500  P = 6.000000E+06  V = 1.00000  Q = 1.287837E+09

UOS BLOCK B8  MODEL: SEP  TIME = 337.78
---FLASH OUTLET STREAM 11 :  
KODE = 2  NTRIAL = 0  T =1173.1500  P = 6.000000E+06  V = 1.00000  Q = 0.000000E+00
---FLASH OUTLET STREAM 13 :  
KODE = 2  NTRIAL = 0  T =1173.1500  P = 6.000000E+06  V = 1.00000  Q = 0.000000E+00

UOS BLOCK B4  MODEL: HEATX  TIME = 337.78
SPECIFICATION: COLD OUTLET TEMP  1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 1173.15 PIN=0.60000E+07  TOUT= 422.14 POUT=0.60000E+07
COLD: TIN= 380.78 PIN=0.60000E+07  TOUT= 1143.15 POUT=0.60000E+07
DUTY=0.65583E+08

UOS BLOCK B5  MODEL: HEATX  TIME = 337.78
SPECIFICATION: COLD OUTLET TEMP  1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 1173.15 PIN=0.60000E+07  TOUT= 432.69 POUT=0.60000E+07
COLD: TIN= 380.78 PIN=0.60000E+07  TOUT= 1143.15 POUT=0.60000E+07
DUTY=0.11395E+09

UOS BLOCK B11  MODEL: MIXER  TIME = 337.78
KODE = 1  NO. TEMP ITER = 4  TEMP = 427.852
KPHASE = 1 KODE = 1 T = 427.852  P = 6.000000E+06 Q = 0.000000E+00

UOS BLOCK B12  MODEL: HEATX  TIME = 337.78
SPECIFICATION: HOT OUTLET TEMP 403.15
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 427.85 PIN=0.60000E+07 TOUT= 403.15 POUT=0.60000E+07
COLD: TIN= 293.15 PIN=0.10000E+06 TOUT= 305.96 POUT=0.20000E+06
DUTY=0.57473E+07

UOS BLOCK B6 MODEL: MIXER TIME = 337.78
KODE = 1 NO. TEMP ITER = 1 TEMP = 1143.15
KPHASE = 1 KODE = 1 T = 1143.15 P = 6.000000E+06 Q = 0.000000E+00

CONVERGENCE BLOCK $SOLVER01 METHOD: WEGSTEIN
TIME = 337.78

--FLASH TEAR STREAM ROUT
NO. TEMP ITER = 1 TEMP = 923.149
KODE = 1 NTRIAL = 0 T = 923.1491 P = 2.000000E+07 V = 1.00000 Q = 0.000000E+00

--FLASH TEAR STREAM 9
KODE = 1 NO. TEMP ITER = 1 TEMP = 1143.15
KPHASE = 1 KODE = 1 T = 1143.15 P = 6.000000E+06 Q = 0.000000E+00

--FLASH TEAR STREAM FEEDH20
NO. TEMP ITER = 5 TEMP = 313.090
KODE = 1 NTRIAL = 2 T = 313.0898 P = 200000. V = 0.000000E+00 Q = 0.000000E+00

LOOP $SOLVER01 ITER 3: 2 VARS NOT CONVERGED, MAX ERR/TOL
10000. TIME = 337.78

UOS BLOCK B2 MODEL: HEATX TIME = 337.78
SPECIFICATION: EXCHANGER DUTY 0.23460E+09
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 923.15 PIN=0.20000E+08 TOUT= 759.46 POUT=0.20000E+08
COLD: TIN= 313.09 PIN=0.20000E+06 TOUT= 620.71 POUT=0.16300E+08
DUTY=0.23460E+09

UOS BLOCK REACTOR MODEL: HEATER TIME = 337.80
NO. TEMP ITER = 8 TEMP = 296.178
NO. TEMP ITER = 11 TEMP = 923.149
KODE = 1 NTRIAL = 1 T = 923.1491 P = 2.000000E+07 V = 1.00000 Q = 0.000000E+00
* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B1" (MODEL: "COMPR")

(CMSTIN.9)
FEED STREAM IS BELOW DEW POINT
OUTLET TEMP = 425.1   OUTLET PRES = 0.6000E+07   INDICATED HP = -
0.1012E+08   BRAKE HP = -0.1012E+08
ISENTR TEMP = 416.4   CALC ISENTR EFF = 0.9000   ISENTR HP = -
0.1125E+08   HP = -0.5226E+08

UOS BLOCK B3   MODEL: FSPLIT   TIME = 337.80
KODE = 1   NO. TEMP ITER = 5   TEMP = 425.137
KPHASE = 1   KODE = 1   T = 425.137   P = 6.000000E+06   Q = 0.000000E+00
SPLIT FRACTIONS: 0.36530D+00 0.63470D+00

UOS BLOCK B9   MODEL: HEATER   TIME = 337.80
KODE = 2   NTRIAL = 0   T = 1173.1500   P = 6.000000E+06   V = 1.00000   Q =
6.907713E+06

UOS BLOCK B7   MODEL: RSTOIC   TIME = 337.80
KODE = 2   NTRIAL = 0   T = 1173.1500   P = 6.000000E+06   V = 1.00000   Q =
1.287837E+09

UOS BLOCK B8   MODEL: SEP   TIME = 337.80
---FLASH OUTLET STREAM 11 :
KODE = 2   NTRIAL = 0   T = 1173.1500   P = 6.000000E+06   V = 1.00000   Q =
0.000000E+00
---FLASH OUTLET STREAM 13 :
KODE = 2   NTRIAL = 0   T = 1173.1500   P = 6.000000E+06   V = 1.00000   Q =
0.000000E+00

UOS BLOCK B4   MODEL: HEATX   TIME = 337.80
SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN = 1173.15   PIN = 0.60000E+07   TOUT = 444.39   POUT = 0.60000E+07
COLD: TIN = 425.14   PIN = 0.60000E+07   TOUT = 1143.15   POUT = 0.60000E+07
DUTY = 0.63750E+08

UOS BLOCK B5   MODEL: HEATX   TIME = 337.80
SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN = 1173.15 PIN = 0.60000E+07 TOUT = 453.67 POUT = 0.60000E+07
COLD: TIN = 425.14 PIN = 0.60000E+07 TOUT = 1143.15 POUT = 0.60000E+07
DUTY = 0.11076E+09

UOS BLOCK B11
MODEL: MIXER
TIME = 337.80
KODE = 1 NO. TEMP ITER = 4 TEMP = 449.393
KPHASE = 1 CODE = 1 T = 449.393 P = 6.000000E+06 Q = 0.000000E+00

UOS BLOCK B12
MODEL: HEATX
TIME = 337.80
SPECIFICATION: HOT OUTLET TEMP 403.15
FLOW TYPE: COUNTERCURRENT
HOT: TIN = 449.39 PIN = 0.60000E+07 TOUT = 403.15 POUT = 0.60000E+07
COLD: TIN = 293.15 PIN = 0.10000E+06 TOUT = 317.17 POUT = 0.20000E+06
DUTY = 0.10765E+08

UOS BLOCK B6
MODEL: MIXER
TIME = 337.80
KODE = 1 NO. TEMP ITER = 1 TEMP = 1143.15
KPHASE = 1 CODE = 1 T = 1143.15 P = 6.000000E+06 Q = 0.000000E+00

CONVERGENCE BLOCK SOLVER01
METHOD: WEGSTEIN
TIME = 337.80

--FLASH TEAR STREAM ROUT
NO. TEMP ITER = 1 TEMP = 923.149
KODE = 1 NTRIAL = 0 T = 923.1491 P = 2.000000E+07 V = 1.00000 Q = 0.000000E+00

--FLASH TEAR STREAM 9
KODE = 1 NO. TEMP ITER = 1 TEMP = 1143.15
KPHASE = 1 CODE = 1 T = 1143.15 P = 6.000000E+06 Q = 0.000000E+00

--FLASH TEAR STREAM FEEDH20
NO. TEMP ITER = 5 TEMP = 322.397
KODE = 1 NTRIAL = 2 T = 322.3965 P = 200000. V = 0.000000E+00 Q = 0.000000E+00

LOOP SOLVER01 ITER 4: 1 VARS NOT CONVERGED, MAX ERR/TOL 12.302 TIME = 337.80

UOS BLOCK B2
MODEL: HEATX
TIME = 337.80
SPECIFICATION: EXCHANGER DUTY 0.23460E+09
FLOW TYPE: COUNTERCURRENT
HOT: TIN = 923.15 PIN = 0.20000E+08 TOUT = 759.46 POUT = 0.20000E+08
COLD: TIN= 322.40 PIN=0.20000E+06 TOUT= 620.71 POUT=0.16300E+08
DUTY=0.23460E+09

UOS BLOCK REACTOR MODEL: HEATER
TIME = 337.80
NO. TEMP ITER = 8  TEMP = 296.178
NO. TEMP ITER = 11  TEMP = 923.149
KODE = 1  NTRIAL = 1  T = 923.1491  P = 2.000000E+07  V = 1.00000  Q = 0.000000E+00

UOS BLOCK B1  MODEL: COMPR
TIME = 337.80

* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B1" (MODEL: "COMPR")
(CMSTIN.9)
FEED STREAM IS BELOW DEW POINT
OUTLET TEMP = 452.3  OUTLET PRES = 0.60000E+07  INDICATED HP = -0.9605E+07  BRAKE HP = -0.9605E+07
ISENTR TEMP = 447.5  CALC ISENTR EFF = 0.9000  ISENTR HP = -0.1067E+08  HP = -0.4958E+08

UOS BLOCK B3  MODEL: FSPLIT
TIME = 337.80
KODE = 1  NO. TEMP ITER = 6  TEMP = 452.288
KPHASE = 1  KODE = 1  T = 452.288  P = 6.000000E+06  Q = 0.000000E+00
SPLIT FRACTIONS: 0.36530D+00  0.63470D+00

UOS BLOCK B9  MODEL: HEATER
TIME = 337.80
KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 6.907713E+06

UOS BLOCK B7  MODEL: RSTOIC
TIME = 337.80
KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 1.287837E+09

UOS BLOCK B8  MODEL: SEP
TIME = 337.80
---FLASH OUTLET STREAM 11
KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 0.000000E+00
---FLASH OUTLET STREAM 13
KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 0.000000E+00

UOS BLOCK B4  MODEL: HEATX
TIME = 338.31
SPECIFICATION: COLD OUTLET TEMP  1143.2
FLOW TYPE:  COUNTERCURRENT
HOT:  TIN= 1173.15  PIN=0.600000E+07  TOUT= 465.12  POUT=0.600000E+07
COLD:  TIN= 452.29  PIN=0.600000E+07  TOUT= 1143.15  POUT=0.600000E+07
DUTY=0.62040E+08

UOS BLOCK B5  MODEL: HEATX  TIME = 338.31
SPECIFICATION: COLD OUTLET TEMP  1143.2
FLOW TYPE:  COUNTERCURRENT
HOT:  TIN= 1173.15  PIN=0.600000E+07  TOUT= 473.24  POUT=0.600000E+07
COLD:  TIN= 452.29  PIN=0.600000E+07  TOUT= 1143.15  POUT=0.600000E+07
DUTY=0.10779E+09

UOS BLOCK B11  MODEL: MIXER  TIME = 338.31
KODE = 1  NO. TEMP ITER = 4  TEMP = 469.472
KPHASE = 1  KODE = 1  T = 469.472  P = 6.000000E+06 Q = 0.000000E+00

UOS BLOCK B12  MODEL: HEATX  TIME = 338.31
SPECIFICATION: HOT OUTLET TEMP  403.15
FLOW TYPE:  COUNTERCURRENT
HOT:  TIN= 469.47  PIN=0.600000E+07  TOUT= 403.15  POUT=0.600000E+07
COLD:  TIN= 293.15  PIN=0.100000E+06  TOUT= 327.64  POUT=0.200000E+06
DUTY=0.15448E+08

UOS BLOCK B6  MODEL: MIXER  TIME = 338.31
KODE = 1  NO. TEMP ITER = 1  TEMP = 1143.15
KPHASE = 1  KODE = 1  T = 1143.15  P = 6.000000E+06 Q = 0.000000E+00

CONVERGENCE BLOCK SOLVER01  METHOD: WEGSTEIN
TIME = 338.31

--FLASH TEAR STREAM ROUT
NO. TEMP ITER = 1  TEMP = 923.149
KODE = 1  NTRIAL = 0  T = 923.1491  P = 2.000000E+07  V = 1.00000  Q = 0.000000E+00

--FLASH TEAR STREAM 9
KODE = 1  NO. TEMP ITER = 1  TEMP = 1143.15
KPHASE = 1  KODE = 1  T = 1143.15  P = 6.000000E+06 Q = 0.000000E+00

--FLASH TEAR STREAM FEEDH20
NO. TEMP ITER = 5  TEMP = 327.640
KODE = 1  NTRIAL =  2  T = 327.6397  P = 200000.  V = 0.000000E+00  Q =
0.000000E+00

LOOP $SOLVER01 ITER  5:  1 VARS NOT CONVERGED, MAX ERR/TOL
15.847  TIME =  338.31

UOS BLOCK B2  MODEL: HEATX  TIME =
338.31
SPECIFICATION: EXCHANGER DUTY  0.23460E+09
FLOW TYPE:  COUNTERCURRENT
HOT:  TIN= 923.15  PIN=0.20000E+08  TOUT= 759.46  POUT=0.20000E+08
COLD:  TIN= 327.64  PIN=0.20000E+06  TOUT= 620.71  POUT=0.16300E+08
   DUTY=0.23460E+09

UOS BLOCK REACTOR  MODEL: HEATER  TIME =
338.31
NO. TEMP ITER =  8  TEMP = 296.178
NO. TEMP ITER =  11  TEMP = 923.149
   KODE = 1  NTRIAL =  1  T = 923.1491  P = 2.000000E+07  V = 1.00000  Q =
0.000000E+00

UOS BLOCK B1  MODEL: COMPR  TIME =
338.31

*  WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B1" (MODEL:
"COMPR")
  (CMSTIN.9)
FEED STREAM IS BELOW DEW POINT
OUTLET TEMP = 459.8  OUTLET PRES = 0.60000E+07  INDICATED HP = -
0.9563E+07  BRAKE HP = -0.9563E+07
ISENTR TEMP = 457.0  CALC ISENTR EFF = 0.9000  ISENTR HP = -
0.1063E+08  HP = -0.4937E+08

UOS BLOCK B3  MODEL: FSPLIT  TIME =  338.31
KODE = 1  NO. TEMP ITER =  6  TEMP = 459.758
KPHASE = 1  KODE =  1  T = 459.758  P = 6.000000E+06  Q = 0.000000E+00
SPLIT FRACTIONS:  0.36530D+00  0.63470D+00

UOS BLOCK B9  MODEL: HEATER  TIME =
338.31
KODE = 2  NTRIAL =  0  T =1173.1500  P = 6.000000E+06  V = 1.00000  Q =
6.907713E+06

UOS BLOCK B7  MODEL: RSTOIC  TIME =  338.31
KODE = 2  NTRIAL =  0  T =1173.1500  P = 6.000000E+06  V = 1.00000  Q =
1.287837E+09

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UOS BLOCK B8  MODEL: SEP  TIME = 338.31
---FLASH OUTLET STREAM 11 :
  KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 0.000000E+00
---FLASH OUTLET STREAM 13 :
  KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 0.000000E+00

UOS BLOCK B4  MODEL: HEATX  TIME =
338.31
SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 1173.15  PIN= 0.600000E+07  TOUT= 475.68  POUT= 0.600000E+07
COLD: TIN= 459.76  PIN= 0.600000E+07  TOUT= 1143.15  POUT= 0.600000E+07
DUTY= 0.61167E+08

UOS BLOCK B5  MODEL: HEATX  TIME =
338.31
SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 1173.15  PIN= 0.600000E+07  TOUT= 483.23  POUT= 0.600000E+07
COLD: TIN= 459.76  PIN= 0.600000E+07  TOUT= 1143.15  POUT= 0.600000E+07
DUTY= 0.10628E+09

UOS BLOCK B11  MODEL: MIXER  TIME =
338.31
  KODE = 1  NO. TEMP ITER = 4  TEMP = 479.700
  KPHASE = 1  KODE = 1  T = 479.700  P = 6.000000E+06  Q = 0.000000E+00

UOS BLOCK B12  MODEL: HEATX  TIME =
338.31
SPECIFICATION: HOT OUTLET TEMP 403.15
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 479.70  PIN= 0.600000E+07  TOUT= 403.15  POUT= 0.600000E+07
COLD: TIN= 293.15  PIN= 0.100000E+06  TOUT= 332.97  POUT= 0.200000E+06
DUTY= 0.17836E+08

UOS BLOCK B6  MODEL: MIXER  TIME = 338.31
  KODE = 1  NO. TEMP ITER = 1  TEMP = 1143.15
  KPHASE = 1  KODE = 1  T = 1143.15  P = 6.000000E+06  Q = 0.000000E+00

CONVERGENCE BLOCK SOLVER01 METHOD: WEGSTEIN
TIME = 338.31

--FLASH TEAR STREAM ROUT
NO. TEMP ITER = 1 TEMP = 923.149
KODE = 1 NTRIAL = 0 T = 923.1491 P = 2.000000E+07 V = 1.00000 Q =
0.000000E+00

--FLASH TEAR STREAM 9
KODE = 1 NO. TEMP ITER = 1 TEMP = 1143.15
KPHASE = 1 KODE = 1 T = 1143.15 P = 6.000000E+06 Q = 0.000000E+00

--FLASH TEAR STREAM FEEDH2O
NO. TEMP ITER = 5 TEMP = 332.974
KODE = 1 NTRIAL = 2 T = 332.9744 P = 200000. V = 0.000000E+00 Q =
0.000000E+00

LOOP $OLVER01 ITER 6: 1 VARS NOT CONVERGED, MAX ERR/TOL
16.155 TIME = 338.33

UOS BLOCK B2 MODEL: HEATX TIME = 338.33
SPECIFICATION: EXCHANGER DUTY 0.23460E+09
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 923.15 PIN=0.20000E+08 TOUT= 759.46 POUT=0.20000E+08
COLD: TIN= 332.97 PIN=0.20000E+06 TOUT= 620.71 POUT=0.16300E+08
DUTY=0.23460E+09

UOS BLOCK REACTOR MODEL: HEATER TIME = 338.33
NO. TEMP ITER = 8 TEMP = 296.178
NO. TEMP ITER = 11 TEMP = 923.149
KODE = 1 NTRIAL = 1 T = 923.1491 P = 2.000000E+07 V = 1.00000 Q =
0.000000E+00

UOS BLOCK B1 MODEL: COMPR TIME = 338.33

* WARNING WHILE EXECUTING UNIT OPERATIONS BLOCK: "B1" (MODEL:
"COMPR")
(COMSTIN.9)
FEED STREAM IS BELOW DEW POINT
OUTLET TEMP = 461.9 OUTLET PRES = 0.60000E+07 INDICATED HP = -
0.9802E+07 BRAKE HP = -0.9802E+07
ISENTR TEMP = 461.4 CALC ISENTR EFF = 0.9000 ISENTR HP = -
0.1089E+08 HP = -0.5060E+08

UOS BLOCK B3 MODEL: FSPLIT TIME = 338.33
KODE = 1 NO. TEMP ITER = 13 TEMP = 461.938
KPHASE = 1 KODE = 1 T = 461.938 P = 6.000000E+06 Q = 0.000000E+00
SPLIT FRACTIONS: 0.36530D+00  0.63470D+00

UOS BLOCK B9  MODEL: HEATER  TIME = 338.33
  KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 6.907713E+06

UOS BLOCK B7  MODEL: RSTOIC  TIME = 338.33
  KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 1.287837E+09

UOS BLOCK B8  MODEL: SEP  TIME = 338.33
  ---FLASH OUTLET STREAM 11:
    KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 0.000000E+00
  ---FLASH OUTLET STREAM 13:
    KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 0.000000E+00

UOS BLOCK B4  MODEL: HEATX  TIME = 338.33
  SPECIFICATION: COLD OUTLET TEMP  1143.2
  FLOW TYPE: COUNTERCURRENT
  HOT: TIN = 1173.15  PIN = 0.600000E+07  TOUT = 485.17  POUT = 0.600000E+07
  COLD: TIN = 461.94  PIN = 0.600000E+07  TOUT = 1143.15  POUT = 0.600000E+07
  DUTY = 0.60382E+08

UOS BLOCK B5  MODEL: HEATX  TIME = 338.33
  SPECIFICATION: COLD OUTLET TEMP  1143.2
  FLOW TYPE: COUNTERCURRENT
  HOT: TIN = 1173.15  PIN = 0.600000E+07  TOUT = 492.21  POUT = 0.600000E+07
  COLD: TIN = 461.94  PIN = 0.600000E+07  TOUT = 1143.15  POUT = 0.600000E+07
  DUTY = 0.10491E+09

UOS BLOCK B11  MODEL: MIXER  TIME = 338.33
  KODE = 1  NO. TEMP ITER = 4  TEM = 488.901
  KPHASE = 1  KODE = 1  T = 488.901  P = 6.000000E+06  Q = 0.000000E+00

UOS BLOCK B12  MODEL: HEATX  TIME = 339.20
  SPECIFICATION: HOT OUTLET TEMP  403.15
  FLOW TYPE: COUNTERCURRENT
  HOT: TIN = 488.90  PIN = 0.600000E+07  TOUT = 403.15  POUT = 0.600000E+07
  COLD: TIN = 293.15  PIN = 0.100000E+06  TOUT = 337.77  POUT = 0.200000E+06
DUTY=0.19985E+08

UOS BLOCK B6  MODEL: MIXER
KODE = 1  NO. TEMP ITER = 1  TEMP = 1143.15
KPHASE = 1  KODE = 1  T = 1143.15  P = 6.000000E+06  Q = 0.000000E+00

CONVERGENCE BLOCK SOLVER01 METHOD: WEGSTEIN
TIME = 339.20

--FLASH TEAR STREAM ROUT
NO. TEMP ITER = 1  TEMP = 923.149
KODE = 1  NTRIAL = 0  T = 923.1491  P = 2.000000E+07  V = 1.00000  Q = 0.000000E+00

--FLASH TEAR STREAM 9
KODE = 1  NO. TEMP ITER = 1  TEMP = 1143.15
KPHASE = 1  KODE = 1  T = 1143.15  P = 6.000000E+06  Q = 0.000000E+00

--FLASH TEAR STREAM FEEDH20
NO. TEMP ITER = 4  TEMP = 361.701
KODE = 1  NTRIAL = 2  T = 361.7005  P = 200000.  V = 0.000000E+00  Q = 0.000000E+00

LOOP SOLVER01 ITER 7: 1 VARS NOT CONVERGED, MAX ERR/TOL
14.565 TIME = 339.20

UOS BLOCK B2  MODEL: HEATX
TIME = 339.20
SPECIFICATION: EXCHANGER DUTY 0.23460E+09
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 923.15  PIN=0.20000E+08  TOUT= 759.46  POUT=0.20000E+08
COLD: TIN= 361.70  PIN=0.20000E+06  TOUT= 627.71  POUT=0.16300E+08
DUTY=0.23460E+09

UOS BLOCK REACTOR MODEL: HEATER
TIME = 339.20
NO. TEMP ITER = 8  TEMP = 296.178
NO. TEMP ITER = 11  TEMP = 923.149
KODE = 1  NTRIAL = 1  T = 923.1491  P = 2.000000E+07  V = 1.00000  Q = 0.000000E+00

UOS BLOCK B1  MODEL: COMPR
TIME = 339.20
OUTLET TEMP = 474.5  OUTLET PRES = 0.60000E+07  INDICATED HP = -0.1265E+08  BRAKE HP = -0.1265E+08

177
ISENTR TEMP = 471.5  CALC ISENTR EFF = 0.9000  ISENTR HP = -0.1406E+08 HP = -0.6530E+08

UOS BLOCK B3  MODEL: FSPLIT  TIME = 339.20
KODE = 1  NO. TEMP ITER = 6  TEMP = 474.476
KPHASE = 1  KODE = 1  T = 474.476  P = 6.000000E+06  Q = 0.000000E+00
SPLIT FRACTIONS: 0.36530D+00  0.63470D+00

UOS BLOCK B9  MODEL: HEATER  TIME = 339.20
KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 6.907713E+06

UOS BLOCK B7  MODEL: RSTOIC  TIME = 339.20
KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 1.287837E+09

UOS BLOCK B8  MODEL: SEP  TIME = 339.20
---FLASH OUTLET STREAM 11 :
KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 0.000000E+00
---FLASH OUTLET STREAM 13 :
KODE = 2  NTRIAL = 0  T = 1173.1500  P = 6.000000E+06  V = 1.00000  Q = 0.000000E+00

UOS BLOCK B4  MODEL: HEATX  TIME = 339.20
SPECIFICATION: COLD OUTLET TEMP  1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 1173.15  PIN=0.600000E+07  TOUT= 529.36  POUT=0.600000E+07
COLD: TIN= 474.48  PIN=0.600000E+07  TOUT= 1143.15  POUT=0.600000E+07
DUTY = 0.56712E+08

UOS BLOCK B5  MODEL: HEATX  TIME = 339.20
SPECIFICATION: COLD OUTLET TEMP  1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 1173.15  PIN=0.600000E+07  TOUT= 534.23  POUT=0.600000E+07
COLD: TIN= 474.48  PIN=0.600000E+07  TOUT= 1143.15  POUT=0.600000E+07
DUTY = 0.98536E+08

UOS BLOCK B11  MODEL: MIXER  TIME = 339.20
KODE = 1  NO. TEMP ITER = 4  TEMP = 531.837
KPHASE = 1  KODE = 1  T = 531.837  P = 6.000000E+06  Q = 0.000000E+00
UOS BLOCK B12  MODEL: HEATX  TIME = 339.20
SPECIFICATION: HOT OUTLET TEMP  403.15
FLOW TYPE:  COUNTERCURRENT
HOT: TIN= 531.84 PIN=0.60000E+07 TOUT= 403.15 POUT=0.60000E+07
COLD: TIN= 293.15 PIN=0.10000E+06 TOUT= 360.15 POUT=0.20000E+06
DUTY=0.30032E+08

UOS BLOCK B6  MODEL: MIXER  TIME = 339.20
KODE = 1  NO. TEMP ITER = 1  TEMP = 1143.15
KPHASE = 1 KODE = 1  T = 1143.15  P = 6.00000E+06 Q = 0.000000E+00

CONVERGENCE BLOCK $OLVER01 METHOD: WEGSTEIN

TIME = 339.20

--FLASH TEAR STREAM ROUT
NO. TEMP ITER = 1  TEMP = 923.149
KODE = 1  NTRIAL = 0  T = 923.1491  P = 2.000000E+07  V = 1.00000  Q = 0.000000E+00

--FLASH TEAR STREAM 9
KODE = 1  NO. TEMP ITER = 1  TEMP = 1143.15
KPHASE = 1 KODE = 1  T = 1143.15  P = 6.000000E+06 Q = 0.000000E+00

--FLASH TEAR STREAM FEEDH20
NO. TEMP ITER = 4  TEMP = 354.668
KODE = 1  NTRIAL = 2  T = 354.6678  P = 200000.  V = 0.000000E+00  Q = 0.000000E+00

LOOP $OLVER01 ITER  8: 1 VARS NOT CONVERGED, MAX ERR/TOL  - 4.7799  TIME = 339.20

UOS BLOCK B2  MODEL: HEATX  TIME = 339.20
SPECIFICATION: EXCHANGER DUTY  0.23460E+09
FLOW TYPE:  COUNTERCURRENT
HOT: TIN= 923.15 PIN=0.20000E+08 TOUT= 759.46 POUT=0.20000E+08
COLD: TIN= 354.67 PIN=0.20000E+06 TOUT= 622.52 POUT=0.16300E+08
DUTY=0.23460E+09

UOS BLOCK REACTOR  MODEL: HEATER  TIME = 339.20
NO. TEMP ITER = 8  TEMP = 296.178
NO. TEMP ITER = 11  TEMP = 923.149
KODE = 1  NTRIAL = 1  T = 923.1491  P = 2.000000E+07  V = 1.00000  Q = 0.000000E+00
UOS BLOCK B1 MODEL: COMPR
TIME = 339.20
OUTLET TEMP = 469.6 OUTLET PRES = 0.6000E+07 INDICATED HP = -
0.1194E+08 BRAKE HP = -0.1194E+08
ISENTR TEMP = 467.3 CALC ISENTR EFF = 0.9000 ISENTR HP = -
0.1327E+08 HP = -0.6164E+08

UOS BLOCK B3 MODEL: FSPLIT TIME = 339.20
KODE = 1 NO. TEMP ITER = 6 TEMP = 469.559
KPHASE = 1 KODE = 1 T = 469.559 P = 6.000000E+06 Q = 0.000000E+00
SPLIT FRACTIONS: 0.36530D+00 0.63470D+00

UOS BLOCK B9 MODEL: HEATER TIME = 339.20
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.000000E+06 V = 1.00000 Q =
6.907713E+06

UOS BLOCK B7 MODEL: RSTOIC TIME = 339.20
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.000000E+06 V = 1.00000 Q =
1.287837E+09

UOS BLOCK B8 MODEL: SEP TIME = 339.20
---FLASH OUTLET STREAM 11 :
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.000000E+06 V = 1.00000 Q =
0.000000E+00
---FLASH OUTLET STREAM 13 :
KODE = 2 NTRIAL = 0 T = 1173.1500 P = 6.000000E+06 V = 1.00000 Q =
0.000000E+00

UOS BLOCK B4 MODEL: HEATX TIME =
339.20
SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN = 1173.15 PIN = 0.60000E+07 TOUT = 518.59 POUT = 0.60000E+07
COLD: TIN = 469.56 PIN = 0.60000E+07 TOUT = 1143.15 POUT = 0.60000E+07
DUTY = 0.57609E+08

UOS BLOCK B5 MODEL: HEATX TIME =
339.20
SPECIFICATION: COLD OUTLET TEMP 1143.2
FLOW TYPE: COUNTERCURRENT
HOT: TIN = 1173.15 PIN = 0.60000E+07 TOUT = 523.96 POUT = 0.60000E+07
COLD: TIN = 469.56 PIN = 0.60000E+07 TOUT = 1143.15 POUT = 0.60000E+07
DUTY = 0.10009E+09
UOS BLOCK B11  MODEL: MIXER  TIME = 339.22
  KODE = 1  NO. TEMP ITER = 4  TEMP = 521.354
  KPHASE = 1  KODE = 1  T = 521.354  P = 6.00000E+06  Q = 0.00000E+00

UOS BLOCK B12  MODEL: HEATX  TIME = 339.22
  SPECIFICATION: HOT OUTLET TEMP  403.15
  FLOW TYPE:  COUNTERCURRENT
  HOT:  TIN = 521.35  PIN = 0.60000E+07  TOUT = 403.15  POUT = 0.60000E+07
  COLD:  TIN = 293.15  PIN = 0.10000E+06  TOUT = 354.69  POUT = 0.20000E+06
     DUTY = 0.27576E+08

UOS BLOCK B6  MODEL: MIXER  TIME = 339.22
  KODE = 1  NO. TEMP ITER = 1  TEMP = 1143.15
  KPHASE = 1  KODE = 1  T = 1143.15  P = 6.00000E+06  Q = 0.00000E+00

CONVERGENCE BLOCK SOLVER01  METHOD: WEGSTEIN
  TIME = 339.22

LOOP $OLVER01 ITER 9:  *** CONVERGED ***, MAX ERR/TOL 0.71119E-01  TIME = 339.22

GENERATING RESULTS FOR UOS BLOCK B2  MODEL: HEATX
  TIME = 340.05
  SPECIFICATION: EXCHANGER DUTY  0.23460E+09
  FLOW TYPE:  COUNTERCURRENT
  HOT:  TIN = 923.15  PIN = 0.20000E+08  TOUT = 759.46  POUT = 0.20000E+08
  COLD:  TIN = 354.69  PIN = 0.20000E+06  TOUT = 622.52  POUT = 0.16300E+06
     AREA = 787.08  DUTY = 0.23460E+09  FT = 1.00000

GENERATING RESULTS FOR UOS BLOCK B4  MODEL: HEATX
  TIME = 340.06
  SPECIFICATION: COLD OUTLET TEMP  1143.2
  FLOW TYPE:  COUNTERCURRENT
  HOT:  TIN = 1173.15  PIN = 0.60000E+07  TOUT = 518.59  POUT = 0.60000E+07
  COLD:  TIN = 469.56  PIN = 0.60000E+07  TOUT = 1143.15  POUT = 0.60000E+07
     AREA = 1749.5  DUTY = 0.57609E+08  FT = 1.00000

GENERATING RESULTS FOR UOS BLOCK B5  MODEL: HEATX
  TIME = 340.06
  SPECIFICATION: COLD OUTLET TEMP  1143.2
  FLOW TYPE:  COUNTERCURRENT
  HOT:  TIN = 1173.15  PIN = 0.60000E+07  TOUT = 523.96  POUT = 0.60000E+07
  COLD:  TIN = 469.56  PIN = 0.60000E+07  TOUT = 1143.15  POUT = 0.60000E+07
     AREA = 2872.4  DUTY = 0.10009E+09  FT = 1.00000
GENERATING RESULTS FOR UOS BLOCK B12 MODEL: HEATX
TIME = 340.06
SPECIFICATION: HOT OUTLET TEMP 403.15
FLOW TYPE: COUNTERCURRENT
HOT: TIN= 521.35 PIN=0.60000E+07 TOUT= 403.15 POUT=0.60000E+07
COLD: TIN= 293.15 PIN=0.10000E+06 TOUT= 354.69 POUT=0.20000E+06
AREA = 237.89 DUTY=0.27576E+08 FT=1.00000

Report Writer entered

Results generated

RUN SAVED

*** SUMMARY OF ERRORS ***

   PHYSICAL
   PROPERTY SYSTEM SIMULATION
TERMINAL ERRORS 0 0 0
SEVERE ERRORS 0 0 0
ERRORS 0 0 4
WARNINGS 0 0 7

Model Report

CONVERGENCE BLOCK: $OLVER01

Tear Stream : ROUT 9 FEEDH20
Tolerance used: 0.100D-03 0.100D-03 0.100D-03
Trace molefrac: 0.100D-05 0.100D-05 0.100D-05

MAXIT= 30 WAIT 1 ITERATIONS BEFORE ACCELERATING
QMAX = 0.00E+00 QMIN = -5.0
METHOD: WEGSTEIN STATUS: CONVERGED
TOTAL NUMBER OF ITERATIONS: 7

*** FINAL VALUES ***

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>VALUE</th>
<th>PREV VALUE</th>
<th>ERR/TOL</th>
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<tr>
<td>TOTAL MOLEFLOW</td>
<td>9.3510+04</td>
<td>9.3510+04</td>
<td>0.0</td>
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<tr>
<td>TOTAL MOLEFLOW</td>
<td>1.8584+04</td>
<td>1.8584+04</td>
<td>0.0</td>
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</table>
TOTAL MOLEFLOW KMOL/HR 1.8584+04 1.8584+04 0.0
CARBO-01MOLEFLOW KMOL/HR 9.3510+04 9.3510+04 0.0
WATER MOLEFLOW KMOL/HR 0.0 0.0 0.0
HYDRO-01MOLEFLOW KMOL/HR 0.0 0.0 0.0
OXYGE-01MOLEFLOW KMOL/HR 0.0 0.0 0.0
PRESSURE BAR 200.0000 200.0000 0.0
MASS ENTHALPY KCAL/KG -1976.7908 -1976.7908 0.0
CARBO-01MOLEFLOW KMOL/HR 0.0 0.0 0.0
WATER MOLEFLOW KMOL/HR 0.0 0.0 0.0
HYDRO-01MOLEFLOW KMOL/HR 0.0 0.0 0.0
OXYGE-01MOLEFLOW KMOL/HR 0.0 0.0 0.0
PRESSURE BAR 60.0000 60.0000 0.0
MASS ENTHALPY KCAL/KG -2787.8036 -2787.8036 0.0
CARBO-01MOLEFLOW KMOL/HR 0.0 0.0 0.0
WATER MOLEFLOW KMOL/HR 0.0 0.0 0.0
HYDRO-01MOLEFLOW KMOL/HR 0.0 0.0 0.0
OXYGE-01MOLEFLOW KMOL/HR 0.0 0.0 0.0
PRESSURE BAR 2.0000 2.0000 0.0
MASS ENTHALPY KCAL/KG -3764.5541 -3764.5557 4.3042-03

*** ITERATION HISTORY ***

TEAR STREAMS:

ITERATION MAX-ERR/TOL STREAM ID VARIABLE
------- ---------- ------- -------
 1 0.1000E+07  9      PRESSURE
 2 0.1000E+05 FEEDH20 PRESSURE
 3 15.31  FEEDH20 MASS ENTHALPY
 4 12.59  FEEDH20 MASS ENTHALPY
 5 10.46  FEEDH20 MASS ENTHALPY
 6 -3.625 FEEDH20 MASS ENTHALPY
 7 0.4304E-02 FEEDH20 MASS ENTHALPY

1 10 11 13 14
-------

STREAM ID  1 10 11 13 14
FROM :  B2 B7 B8 B8 B11
TO :   B1 B8 B4 B5 B12

SUBSTREAM: MIXED
PHASE: VAPOR VAPOR VAPOR VAPOR VAPOR
COMPONENTS: KMOL/HR
CARBO-01 0.0 0.0 0.0 0.0 0.0
| WATER      | 1.8584E+04 0.0 0.0 0.0 0.0 |
| HYDRO-01  | 0.0 1.8584E+04 0.0 1.8584E+04 1.8584E+04 |
| OXYGE-01  | 0.0 9292.1120 9292.1120 0.0 9292.1120 |
| COMPONENTS: KG/HR |
| CARBO-01  | 0.0 0.0 0.0 0.0 0.0 |
| WATER     | 3.3480E+05 0.0 0.0 0.0 0.0 |
| HYDRO-01  | 0.0 3.7464E+04 0.0 3.7464E+04 3.7464E+04 |
| OXYGE-01  | 0.0 2.9734E+05 2.9734E+05 0.0 2.9734E+05 |
| TOTAL FLOW: |
| KMOL/HR   | 1.8584E+04 2.7876E+04 9292.1120 1.8584E+04 2.7876E+04 |
| KG/HR     | 3.3480E+05 3.3480E+05 2.9734E+05 3.7464E+04 3.3480E+05 |
| CUM/HR    | 3441.4496 4.5860E+04 1.5310E+04 3.0550E+04 2.0640E+04 |
| STATE VARIABLES: |
| TEMP C    | 349.4406 900.0000 900.0000 900.0000 248.3487 |
| PRES BAR  | 163.0000 60.0000 60.0000 60.0000 60.0000 |
| VFRAC     | 1.0000 1.0000 1.0000 1.0000 1.0000 |
| LFRAC     | 0.0 0.0 0.0 0.0 0.0 |
| SFRACT    | 0.0 0.0 0.0 0.0 0.0 |
| ENTHALPY: |
| KCAL/MOL  | -56.9652 6.4544 6.9086 6.2270 1.5908 |
| KCAL/KG   | -3162.0477 537.4065 215.9005 3088.9740 132.4580 |
| MMKCAL/HR | -1058.6688 179.9263 64.1960 115.7256 44.3476 |
| ENTROPY: |
| CAL/MOL-K | -16.9918 3.0990 2.4134 1.5456 -2.9226 |
| CAL/GM-K  | -0.9432 0.2580 7.5423-02 0.7667 -0.2433 |
| DENSITY: |
| KMOL/CUM  | 5.4001 0.6079 0.6069 0.6083 1.3506 |
| KG/CUM    | 97.2846 7.3004 19.4210 1.2263 16.2211 |
| AVG MW    | 18.0153 12.0102 31.9988 2.0159 12.0102 |

15 16 17 2 5
--------

| STREAM ID | 15 | 16 | 17 | 2 | 5 |
| FROM :    | B9 | B12 | ---- | B1 | B3 |
| TO :      | B7 | ---- | B12 | B3 | B4 |

SUBSTREAM: MIXED
PHASE: VAPOR VAPOR LIQUID VAPOR VAPOR
COMPONENTS: KMOL/HR
| CARBO-01  | 0.0 0.0 0.0 0.0 0.0 |
| WATER     | 1.8584E+04 0.0 1.8584E+04 1.8584E+04 6788.8170 |
| HYDRO-01  | 0.0 1.8584E+04 0.0 0.0 0.0 |
| OXYGE-01  | 0.0 9292.1120 0.0 0.0 0.0 |
| COMPONENTS: KG/HR |
| CARBO-01  | 0.0 0.0 0.0 0.0 0.0 |
### Total Flow

<table>
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<tr>
<th>Flow Type</th>
<th>KMOL/HR</th>
<th>KG/HR</th>
<th>CUM/HR</th>
</tr>
</thead>
<tbody>
<tr>
<td>WATER</td>
<td>3.3480+05</td>
<td>3.3480+05</td>
<td>3.3480+05</td>
</tr>
<tr>
<td>HYDRO-01</td>
<td>0.0</td>
<td>3.7464+04</td>
<td>0.0</td>
</tr>
<tr>
<td>OXYGE-01</td>
<td>0.0</td>
<td>2.9734+05</td>
<td>0.0</td>
</tr>
</tbody>
</table>

### State Variables

<table>
<thead>
<tr>
<th>State Variable</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>TEMP C</td>
<td>°C</td>
<td>900.0000</td>
</tr>
<tr>
<td>PRES BAR</td>
<td>Bar</td>
<td>60.0000</td>
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<tr>
<td>VFRAC</td>
<td></td>
<td>1.0000</td>
</tr>
<tr>
<td>LFRAC</td>
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<td>0.0000</td>
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<tr>
<td>SFRAC</td>
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<td>0.0000</td>
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### Enthalpy

<table>
<thead>
<tr>
<th>Component</th>
<th>KCAL/MOL</th>
<th>KCAL/KG</th>
<th>MMKCAL/HR</th>
</tr>
</thead>
<tbody>
<tr>
<td>WATER</td>
<td>-49.9035</td>
<td>-69.0969</td>
<td>-57.5181</td>
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### Entropy

<table>
<thead>
<tr>
<th>Component</th>
<th>CAL/MOL-K</th>
<th>CAL/GM-K</th>
<th>MMKCAL/HR</th>
</tr>
</thead>
<tbody>
<tr>
<td>WATER</td>
<td>-6.6905</td>
<td>-0.3714</td>
<td>-0.3975</td>
</tr>
</tbody>
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### Density

<table>
<thead>
<tr>
<th>Component</th>
<th>KMOL/CUM</th>
<th>KG/CUM</th>
<th>AVG MW</th>
</tr>
</thead>
<tbody>
<tr>
<td>WATER</td>
<td>0.6152</td>
<td>11.0837</td>
<td>18.0153</td>
</tr>
</tbody>
</table>

### Stream ID

<table>
<thead>
<tr>
<th>Stream ID</th>
<th>From</th>
<th>To</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 7 8 9</td>
<td>B4 B3 B5 B6 B12</td>
<td>B6 B5 B6 B9 B2</td>
</tr>
</tbody>
</table>

### Max Conv. Error

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
</tr>
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<tbody>
<tr>
<td>WATER</td>
<td>4.3042-07</td>
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</tbody>
</table>

### Substream: Mixed

### Phase: VAPOR VAPOR VAPOR VAPOR LIQUID

### Components: KMOL/HR

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CARBO-01</td>
<td>0.0</td>
</tr>
<tr>
<td>WATER</td>
<td>6788.8170</td>
</tr>
<tr>
<td>HYDRO-01</td>
<td>0.0</td>
</tr>
<tr>
<td>OXYGE-01</td>
<td>0.0</td>
</tr>
</tbody>
</table>

### Components: KG/HR

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>CARBO-01</td>
<td>0.0</td>
</tr>
<tr>
<td>WATER</td>
<td>1.2230+05</td>
</tr>
<tr>
<td>HYDRO-01</td>
<td>0.0</td>
</tr>
<tr>
<td>OXYGE-01</td>
<td>0.0</td>
</tr>
</tbody>
</table>

---

6789 FEEDH20
TOTAL FLOW:
KMOL/HR  6788.8170  1.1795+04  1.1795+04  1.8584+04  1.8584+04
KG/HR  1.2230+05  2.1250+05  2.1250+05  3.3480+05  3.3480+05
CUM/HR  1.0739+04  4538.2126  1.8658+04  2.9397+04  463.5010
STATE VARIABLES:
TEMP C  870.0000  196.4704  870.0000  870.0000  81.6163
PRES BAR  60.0000  60.0000  60.0000  60.0000  2.0000
VFRAC  0.0  0.0  0.0  0.0  1.0000
LFRAC  0.0  0.0  0.0  0.0  0.0
SFRAC  0.0  0.0  0.0  0.0  0.0
ENTHALPY:
KCAL/KG  -2787.8036  -3192.7382  -2787.8036  -2787.8036  -3764.5541
MMKCAL/HR  -340.9601  -678.4588  -592.4100  -933.3700  -1260.3908
ENTROPY:
CAL/GM-K  -0.3867  -0.9359  -0.3867  -0.3867  -2.0651
DENSITY:
KMOL/CUM  0.6322  2.5991  0.6322  0.6322  40.0953
KG/CUM  11.3889  46.8241  11.3889  11.3889  722.3285
AVG MW  18.0153  18.0153  18.0153  18.0153  18.0153

H2 O2 RIN ROUT
-------------
STREAM ID   H2   O2   RIN   ROUT
FROM :      B5   B4   B2   REACTOR
TO :        B11  B11  REACTOR  B2

SUBSTREAM: MIXED
PHASE:       VAPOR VAPOR VAPOR VAPOR VAPOR
COMPONENTS: KMOL/HR
CARBO-01    0.0  0.0  9.3510+04  9.3510+04
WATER       0.0  0.0  0.0  0.0
HYDRO-01    1.8584+04  0.0  0.0  0.0
OXYGE-01    0.0  9292.1120  0.0  0.0

COMPONENTS: KG/HR
CARBO-01    0.0  0.0  4.1153+06  4.1153+06
WATER       0.0  0.0  0.0  0.0
HYDRO-01    3.7464+04  0.0  0.0  0.0
OXYGE-01    0.0  2.9734+05  0.0  0.0

TOTAL FLOW:
KMOL/HR  1.8584+04  9292.1120  9.3510+04  9.3510+04
KG/HR  3.7464+04  2.9734+05  4.1153+06  4.1153+06
CUM/HR  1.3827+04  6821.4645  3.1373+04  3.8262+04
STATE VARIABLES:
TEMP C  250.9490  245.5896  486.3125  649.9991
PRES BAR  60.0000  60.0000  200.0000  200.0000
VFRAC   1.0000  1.0000  1.0000  1.0000
LFRAC   0.0  0.0  0.0  0.0
SFRAC   0.0  0.0  0.0  0.0
ENTHALPY:
    KCAL/MOL   1.5969  1.5788  -89.1554  -86.9982
    KCAL/KG    792.1392  49.3400  -2025.8073  -1976.7908
    MMKCAL/HR  29.6768  14.6708  -8337.0200  -8135.2974
ENTROPY:
    CAL/MOL-K  -4.1832  -4.1868  -0.2636  2.3082
    CAL/GM-K   -2.0751  -0.1308  -5.9892E-03  5.2448E-02
DENSITY:
    KMOL/CUM   1.3441  1.3622  2.9806  2.4439
    KG/CUM     2.7095  43.5884  131.1763  107.5565
    AVG MW    2.0159  31.9988  44.0098  44.0098

BLOCK: B1  MODEL: COMPR
-----------------------------
INLET STREAM:  1
OUTLET STREAM:  2
PROPERTY OPTION SET: RKS-BM  REDLICH-KWONG-SOAVE EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***
TOTAL BALANCE
IN  OUT  RELATIVE DIFF.

MOLE(KMOL/HR ) 18584.2  18584.2  0.000000E+00
MASS(KG/HR )  334800.  334800.  0.000000E+00
ENTHALPY(MMKCAL/H)  -1058.67  -1068.94  0.961260E-02

*** INPUT DATA ***

GAS PHASE CALCULATION
NO FLASH PERFORMED
ISENTROPIC TURBINE
PRESSURE RATIO  0.36810
ISENTROPIC EFFICIENCY  0.90000
MECHANICAL EFFICIENCY  1.00000

*** RESULTS ***

INDICATED HORSEPOWER REQUIREMENT KW  -11,950.0
BRAKE  HORSEPOWER REQUIREMENT KW  -11,950.0
NET WORK REQUIRED  KW  -11,950.0
POWER LOSSES  KW  0.0
ISENTRIC HORSEPOWER REQUIREMENT KW  -13,277.8
CALCULATED OUTLET PRES  BAR  60.0000
CALCULATED OUTLET TEMP  C  196.470
ISENTRIC TEMPERATURE  C  194.231
EFFICIENCY (POLYTR/ISENTR) USED  0.90000
OUTLET VAPOR FRACTION  1.00000
IDEAL HEAD DEVELOPED, METER  -14,558.7
ACTUAL HEAD DEVELOPED, METER  -13,102.8
MECHANICAL EFFICIENCY USED  1.00000
INLET HEAT CAPACITY RATIO  1.06936
INLET VOLUMETRIC FLOW RATE, CUM/HR  3,441.45
OUTLET VOLUMETRIC FLOW RATE, CUM/HR  7,150.17
INLET COMPRESSIBILITY FACTOR  0.58312
OUTLET COMPRESSIBILITY FACTOR  0.59122
AV. ISENT. VOL. EXPONENT  1.43513
AV. ISENT. TEMP EXPONENT  1.40236
AV. ACTUAL VOL. EXPONENT  1.36672
AV. ACTUAL TEMP EXPONENT  1.39301

BLOCK: B2  MODEL: HEATX

HOT SIDE:

INLET STREAM:  ROUT
OUTLET STREAM:  RIN
PROPERTY OPTION SET:  RKS-BM  REDLICH-KWONG-SOAVE EQUATION
OF STATE
COLD SIDE:

INLET STREAM:  FEEDH20
OUTLET STREAM:  1
PROPERTY OPTION SET:  RKS-BM  REDLICH-KWONG-SOAVE EQUATION
OF STATE

*** MASS AND ENERGY BALANCE ***

IN   OUT    RELATIVE DIFF.

TOTAL BALANCE
MOLE(KMOL/HR )  112094.  112094.  0.000000E+00
MASS(KG/HR )  0.445015E+07  0.445015E+07  0.000000E+00
ENTHALPY(MMKCAL/H)  -9395.69  -9395.69  0.577393E-07

*** INPUT DATA ***

FLASH SPECS FOR HOT SIDE:
TWO PHASE  FLASH
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.0001000

FLASH SPECS FOR COLD SIDE:
TWO PHASE FLASH
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.0001000

FLOW DIRECTION AND SPECIFICATION:
COUNTERCURRENT HEAT EXCHANGER
SPECIFIED EXCHANGER DUTY
SPECIFIED VALUE MMKCAL/HR 201.7226
LMTD CORRECTION FACTOR 1.00000

PRESSURE SPECIFICATION:
HOT SIDE PRESSURE DROP BAR 0.0000
COLD SIDE OUTLET PRESSURE BAR 163.0000

HEAT TRANSFER COEFFICIENT SPECIFICATION:
HOT LIQUID COLD LIQUID KCAL/HR-SQM-K 730.8684
HOT 2-PHASE COLD LIQUID KCAL/HR-SQM-K 730.8684
HOT VAPOR COLD LIQUID KCAL/HR-SQM-K 730.8684
HOT LIQUID COLD 2-PHASE KCAL/HR-SQM-K 730.8684
HOT 2-PHASE COLD 2-PHASE KCAL/HR-SQM-K 730.8684
HOT VAPOR COLD 2-PHASE KCAL/HR-SQM-K 730.8684
HOT LIQUID COLD VAPOR KCAL/HR-SQM-K 730.8684
HOT 2-PHASE COLD VAPOR KCAL/HR-SQM-K 730.8684
HOT VAPOR COLD VAPOR KCAL/HR-SQM-K 730.8684

*** OVERALL RESULTS ***

STREAMS:
---------------------------------------------------------------
<table>
<thead>
<tr>
<th>ROUT</th>
<th>HOT</th>
<th>RIN</th>
</tr>
</thead>
<tbody>
<tr>
<td>T= 6.5000D+02</td>
<td>T= 4.8631D+02</td>
<td></td>
</tr>
<tr>
<td>P= 2.0000D+02</td>
<td>P= 2.0000D+02</td>
<td></td>
</tr>
<tr>
<td>V= 1.0000D+00</td>
<td>V= 1.0000D+00</td>
<td></td>
</tr>
<tr>
<td>&lt;-------</td>
<td>&lt;-----</td>
<td></td>
</tr>
<tr>
<td>COLD</td>
<td>FEEDH20</td>
<td></td>
</tr>
<tr>
<td>T= 3.4944D+02</td>
<td>T= 8.1616D+01</td>
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</tr>
<tr>
<td>P= 1.6300D+02</td>
<td>P= 2.0000D+00</td>
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</tr>
<tr>
<td>V= 1.0000D+00</td>
<td>V= 0.0000D+00</td>
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</tbody>
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DUTY AND AREA:
CALCULATED HEAT DUTY MMKCAL/HR 201.7226
CALCULATED (REQUIRED) AREA SQM 787.1936
ACTUAL EXCHANGER AREA SQM 787.1936
PER CENT OVER-DESIGN 0.0000

HEAT TRANSFER COEFFICIENT:
AVERAGE COEFFICIENT (DIRTY) KCAL/HR-SQM-K 730.8684
UA (DIRTY) CAL/SEC-K 159815.2714

LOG-MEAN TEMPERATURE DIFFERENCE:
LMTD CORRECTION FACTOR 1.0000
LMTD (CORRECTED) C 350.6126
NUMBER OF SHELLS IN SERIES 1

PRESSURE DROP:
HOTSIDE, TOTAL BAR 0.0000
COLDSIDE, TOTAL BAR -161.0000

PRESSURE DROP PARAMETER:
HOT SIDE: 0.00000E+00
COLD SIDE: -0.31920E+06

*** ZONE RESULTS ***

TEMPERATURE LEAVING EACH ZONE:

HOT

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
</table>
ROUT | VAP | VAP | RIN |
-------|-----|-----|-----|
650.0 | 649.2 | 486.3 |
1 | VAP | BOIL | FEEDH20 |
<----- | | | <----- |
349.4 | 347.2 | 81.6 |

COLD

ZONE HEAT TRANSFER AND AREA:

<table>
<thead>
<tr>
<th>ZONE</th>
<th>HEAT DUTY MMKCAL/HR</th>
<th>AREA SQM</th>
<th>DTLM</th>
<th>AVERAGE U</th>
<th>UA KCAL/HR-SQM-K</th>
<th>UA CAL/SEC-K</th>
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<tbody>
<tr>
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<td>2</td>
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<td>350.8846</td>
<td>730.8684</td>
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</table>
BLOCK: B3 MODEL: FSPLIT

-----------
INLET STREAM: 2
OUTLET STREAMS: 5 7
PROPERTY OPTION SET: RKS-BM REDLICH-KWONG-SOAVE EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th>TOTAL BALANCE</th>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLE(KMOL/HR)</td>
<td>18584.2</td>
<td>18584.2</td>
<td>0.000000E+00</td>
</tr>
<tr>
<td>MASS(KG/HR)</td>
<td>334800.</td>
<td>334800.</td>
<td>0.000000E+00</td>
</tr>
<tr>
<td>ENTHALPY(MMKCAL/H)</td>
<td>-1068.94</td>
<td>-1068.94</td>
<td>0.000000E+00</td>
</tr>
</tbody>
</table>

*** INPUT DATA ***

OUTLET PRESSURE BAR 60.0000

FRACTION OF FLOW STRM=5 FRAC= 0.36530

*** RESULTS ***

STREAM= 5 SPLIT= 0.36530 KEY= 0 STREAM-ORDER= 1
7 0.63470 0 2

BLOCK: B4 MODEL: HEATX

---------
HOT SIDE:
---------
INLET STREAM: 11
OUTLET STREAM: O2
PROPERTY OPTION SET: RKS-BM REDLICH-KWONG-SOAVE EQUATION OF STATE
COLD SIDE:
---------
INLET STREAM: 5
OUTLET STREAM: 6
PROPERTY OPTION SET: RKS-BM REDLICH-KWONG-SOAVE EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th>TOTAL BALANCE</th>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLE(KMOL/HR)</td>
<td>16080.9</td>
<td>16080.9</td>
<td>0.000000E+00</td>
</tr>
</tbody>
</table>
MASS (KG/HR)  419639.  419639.  0.000000E+00  
ENTHALPY (MMKCAL/H)  -326.289  -326.289  -0.174212E-15

*** INPUT DATA ***

FLASH SPECS FOR HOT SIDE:
TWO PHASE FLASH
MAXIMUM NO. ITERATIONS  30
CONVERGENCE TOLERANCE  0.00010000

FLASH SPECS FOR COLD SIDE:
TWO PHASE FLASH
MAXIMUM NO. ITERATIONS  30
CONVERGENCE TOLERANCE  0.00010000

FLOW DIRECTION AND SPECIFICATION:
COUNTERCURRENT HEAT EXCHANGER
SPECIFIED COLD OUTLET TEMP
SPECIFIED VALUE   C  870.0000
LMTD CORRECTION FACTOR  1.00000

PRESSURE SPECIFICATION:
HOT SIDE PRESSURE DROP   BAR  0.0000
COLD SIDE PRESSURE DROP   BAR  0.0000

HEAT TRANSFER COEFFICIENT SPECIFICATION:
HOT LIQUID COLD LIQUID KCAL/HR-SQM-K  730.8684
HOT 2-PHASE COLD LIQUID KCAL/HR-SQM-K  730.8684
HOT VAPOR COLD LIQUID KCAL/HR-SQM-K  730.8684
HOT LIQUID COLD 2-PHASE KCAL/HR-SQM-K  730.8684
HOT 2-PHASE COLD 2-PHASE KCAL/HR-SQM-K  730.8684
HOT VAPOR COLD 2-PHASE KCAL/HR-SQM-K  730.8684
HOT LIQUID COLD VAPOR KCAL/HR-SQM-K  730.8684
HOT 2-PHASE COLD VAPOR KCAL/HR-SQM-K  730.8684
HOT VAPOR COLD VAPOR KCAL/HR-SQM-K  730.8684

*** OVERALL RESULTS ***

STREAMS:
-----------------------------------------------------------------------------
                  |                      |   |
11     -----|        HOT      |----- O2
                  |                      |
T=  9.0000D+02 | T=  2.4559D+02
P=  6.0000D+01 | P=  6.0000D+01
V=  1.0000D+00 | V=  1.0000D+00
DUTY AND AREA:
CALCULATED HEAT DUTY MMKCAL/HR 49.5252
CALCULATED (REQUIRED) AREA SQM 1747.4475
ACTUAL EXCHANGER AREA SQM 1747.4475
PER CENT OVER-DESIGN 0.0000

HEAT TRANSFER COEFFICIENT:
AVERAGE COEFFICIENT (DIRTY) KCAL/HR-SQM-K 730.8684
UA (DIRTY) CAL/SEC-K 354765.0737

LOG-MEAN TEMPERATURE DIFFERENCE:
LMTD CORRECTION FACTOR 1.0000
LMTD (CORRECTED) C 38.7772
NUMBER OF SHELLS IN SERIES 1

PRESSURE DROP:
HOTSIDE, TOTAL BAR 0.0000
COLD SIDE, TOTAL BAR 0.0000

PRESSURE DROP PARAMETER:
HOT SIDE: 0.00000E+00
COLD SIDE: 0.00000E+00

*** ZONE RESULTS ***

TEMPERATURE LEAVING EACH ZONE:

HOT

<table>
<thead>
<tr>
<th>VAP</th>
<th>O2</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>900.0</td>
</tr>
<tr>
<td>6</td>
<td>870.0</td>
</tr>
</tbody>
</table>

COLD
ZONE HEAT TRANSFER AND AREA:

ZONE    HEAT DUTY   AREA   DTLM   AVERAGE U   UA
       MMKCAL/HR   SQM  C   KCAL/HR-SQM-K   CAL/SEC-K
  1    49.525    1747.475  38.7772   730.8684   354765.0737

BLOCK: B5   MODEL: HEATX

HOT SIDE:

INLET STREAM:  13
OUTLET STREAM: H2
PROPERTY OPTION SET: RKS-BM REDLICH-KWONG-SOAVE EQUATION
OF STATE

COLD SIDE:

INLET STREAM:  7
OUTLET STREAM: 8
PROPERTY OPTION SET: RKS-BM REDLICH-KWONG-SOAVE EQUATION
OF STATE

*** MASS AND ENERGY BALANCE ***

IN     OUT   RELATIVE DIFF.
TOTAL BALANCE
MOLE(KMOL/HR )  30379.6  30379.6   0.000000E+00
MASS(KG/HR )   249961.  249961.   0.000000E+00
ENTHALPY(MMKCAL/H) -562.733  -562.733   0.000000E+00

*** INPUT DATA ***

FLASH SPECS FOR HOT SIDE:
TWO PHASE FLASH
MAXIMUM NO. ITERATIONS  30
CONVERGENCE TOLERANCE   0.00010000

FLASH SPECS FOR COLD SIDE:
TWO PHASE FLASH
MAXIMUM NO. ITERATIONS  30
CONVERGENCE TOLERANCE   0.00010000

FLOW DIRECTION AND SPECIFICATION:
COUNTERCURRENT HEAT EXCHANGER
SPECIFIED COLD OUTLET TEMP
SPECIFIED VALUE C  870.0000
LMTD CORRECTION FACTOR 1.00000

PRESSURE SPECIFICATION:
HOT SIDE PRESSURE DROP BAR 0.0000
COLD SIDE PRESSURE DROP BAR 0.0000

HEAT TRANSFER COEFFICIENT SPECIFICATION:
HOT LIQUID COLD LIQUID KCAL/HR-SQM-K 730.8684
HOT 2-PHASE COLD LIQUID KCAL/HR-SQM-K 730.8684
HOT VAPOR COLD LIQUID KCAL/HR-SQM-K 730.8684
HOT LIQUID COLD 2-PHASE KCAL/HR-SQM-K 730.8684
HOT 2-PHASE COLD 2-PHASE KCAL/HR-SQM-K 730.8684
HOT VAPOR COLD 2-PHASE KCAL/HR-SQM-K 730.8684
HOT LIQUID COLD VAPOR KCAL/HR-SQM-K 730.8684
HOT 2-PHASE COLD VAPOR KCAL/HR-SQM-K 730.8684
HOT VAPOR COLD VAPOR KCAL/HR-SQM-K 730.8684

*** OVERALL RESULTS ***

STREAMS:

| 13 --->| HOT | 8 <-----| COLD |
| T= 9.0000D+02 | T= 2.5095D+02 |
| P= 6.0000D+01 | P= 6.0000D+01 |
| V= 1.0000D+00 | V= 1.0000D+00 |

DUTY AND AREA:
CALCULATED HEAT DUTY MMKCAL/HR 86.0489
CALCULATED (REQUIRED) AREA SQM 2869.4836
ACTUAL EXCHANGER AREA SQM 2869.4836
PER CENT OVER-DESIGN 0.0000

HEAT TRANSFER COEFFICIENT:
AVERAGE COEFFICIENT (DIRTY) KCAL/HR-SQM-K 730.8684
UA (DIRTY) CAL/SEC-K 582559.7199

LOG-MEAN TEMPERATURE DIFFERENCE:
LMTD CORRECTION FACTOR 1.0000
LMTD (CORRECTED) C 41.0295
NUMBER OF SHELLS IN SERIES 1

PRESSURE DROP:
HOTSIDE, TOTAL      BAR        0.0000
COLDSDIE, TOTAL      BAR        0.0000

PRESSURE DROP PARAMETER:
HOT SIDE:            0.00000E+00
COLD SIDE:           0.00000E+00

*** ZONE RESULTS ***

TEMPERATURE LEAVING EACH ZONE:

<table>
<thead>
<tr>
<th>HOT</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>13 VAP H2</td>
<td></td>
</tr>
<tr>
<td>900.0</td>
<td>250.9</td>
</tr>
<tr>
<td>8 VAP 7</td>
<td>196.5</td>
</tr>
</tbody>
</table>

COLD

ZONE HEAT TRANSFER AND AREA:

<table>
<thead>
<tr>
<th>ZONE</th>
<th>HEAT DUTY</th>
<th>AREA</th>
<th>DTLM</th>
<th>AVERAGE U</th>
<th>UA</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>MMKCAL/HR</td>
<td>SQM</td>
<td>C</td>
<td>KCAL/HR-SQM-K</td>
<td>CAL/SEC-K</td>
</tr>
<tr>
<td>1</td>
<td>86.049</td>
<td>2869.4836</td>
<td>41.0295</td>
<td>730.8684</td>
<td>582559.7199</td>
</tr>
</tbody>
</table>

BLOCK: B6 MODEL: MIXER

INLET STREAMS: 6 8
OUTLET STREAM: 9
PROPERTY OPTION SET: RKS-BM REDLICH-KWONG-SOAVE EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th>TOTAL BALANCE</th>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLE(KMOL/HR)</td>
<td>18584.2</td>
<td>18584.2</td>
<td>0.000000E+00</td>
</tr>
</tbody>
</table>
**Input Data**

One Phase Flash Specified

**Maximum Number of Iterations:** 30

**Convergence Tolerance:** 0.00010000

**Outlet Pressure (Bar):** 60.0000

**Block:** B7  **Model:** RSTOIC

**Inlet Stream:** 15  **Outlet Stream:** 10

**Property Option Set:** RKS-BM REDLICH-KWONG-SOAVE Equation of State

**Mass and Energy Balance**

<table>
<thead>
<tr>
<th>Component</th>
<th>In (Moles/hr)</th>
<th>Out (Moles/hr)</th>
<th>Generation (Moles/hr)</th>
<th>Relative Diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mole (Kmol/hr)</td>
<td>18584.2</td>
<td>27876.3</td>
<td>9292.11</td>
<td>0.000000E+00</td>
</tr>
<tr>
<td>Mass (Kg/hr)</td>
<td>334800.0</td>
<td>334800.0</td>
<td>-0.173858E-15</td>
<td></td>
</tr>
<tr>
<td>Enthalpy (MMKCAL/H)</td>
<td>-927.430</td>
<td>179.926</td>
<td>1.19401</td>
<td></td>
</tr>
</tbody>
</table>

**Stoichiometry Matrix:**

Reaction # 1:

Substream Mixed:

- Water: -1.00
- Hydro-01: 1.00
- Oxygen-01: 0.500

**Reaction Conversion Specs:**

Number = 1  Reaction # 1:

Substream: Mixed  Key Component: Water  Conversion: 1.000

**Two Phase TP Flash**

Specified Temperature (C): 900.000

Specified Pressure (Bar): 60.0000

Maximum Number of Iterations: 30

Convergence Tolerance: 0.00010000

Simultaneous Reactions: Generate Combustion Reactions for Feed Species: No
*** RESULTS ***

OUTLET TEMPERATURE  C       900.00
OUTLET PRESSURE    BAR        60.000
HEAT DUTY         MMKCAL/HR  1107.4
VAPOR FRACTION                1.0000

REACTION EXTENTS:

<table>
<thead>
<tr>
<th>REACTION</th>
<th>REACTION NUMBER</th>
<th>EXTENT (KMOL/HR)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>18584.</td>
</tr>
</tbody>
</table>

V-L PHASE EQUILIBRIUM:

<table>
<thead>
<tr>
<th>COMP</th>
<th>F(I)</th>
<th>X(I)</th>
<th>Y(I)</th>
<th>K(I)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HYDRO-01</td>
<td>0.6667</td>
<td>0.6667</td>
<td>0.6667</td>
<td>MISSING</td>
</tr>
<tr>
<td>OXYGE-01</td>
<td>0.3333</td>
<td>0.3333</td>
<td>0.3333</td>
<td>MISSING</td>
</tr>
</tbody>
</table>

BLOCK: B8  MODEL: SEP

Inlet Stream: 10
Outlet Streams: 11 13
Property Option Set: RKS-BM  REDLICH-KWONG-SOAVE EQUATION
OF STATE

*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th></th>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLE</td>
<td>27876.3</td>
<td>27876.3</td>
<td>0.000000E+00</td>
</tr>
<tr>
<td>MASS</td>
<td>334800.3</td>
<td>334800.3</td>
<td>0.173858E-15</td>
</tr>
<tr>
<td>ENTHALPY</td>
<td>179.926</td>
<td>179.922</td>
<td>0.256947E-04</td>
</tr>
</tbody>
</table>

*** INPUT DATA ***

FLASH SPECS FOR STREAM 11
TWO PHASE TP FLASH
PRESSURE DROP BAR 0.0
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.00010000

FLASH SPECS FOR STREAM 13
TWO PHASE TP FLASH
PRESSURE DROP BAR 0.0
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.00010000

FRACTION OF FEED
SUBSTREAM= MIXED
STREAM= 11 CPT= OXYGE-01 FRACTION= 1.00000

*** RESULTS ***

HEAT DUTY MMKCAL/HR -0.46232E-02

COMPONENT = HYDRO-01
STREAM SUBSTREAM SPLIT FRACTION
13 MIXED 1.00000

COMPONENT = OXYGE-01
STREAM SUBSTREAM SPLIT FRACTION
11 MIXED 1.00000

MODEL: HEATER
INLET STREAM: 9
OUTLET STREAM: 15
PROPERTY OPTION SET: RKS-BM REDLICH-KWONG-SOAVE EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

IN OUT RELATIVE DIFF.
TOTAL BALANCE
MOLE(KMOL/HR ) 18584.2 18584.2 0.000000E+00
MASS(KG/HR ) 334800. 334800. 0.000000E+00
ENTHALPY(MMKCAL/H) -933.370 -927.430 -0.636366E-02

*** INPUT DATA ***

TWO PHASE TP FLASH
SPECIFIED TEMPERATURE C 900.000
SPECIFIED PRESSURE BAR 60.0000
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.00010000
*** RESULTS ***
OUTLET TEMPERATURE °C 900.00
OUTLET PRESSURE BAR 60.000
HEAT DUTY MMKCAL/HR 5.9396
OUTLET VAPOR FRACTION 1.0000
PRESSURE-DROP CORRELATION PARAMETER 0.00000E+00

V-L PHASE EQUILIBRIUM:

<table>
<thead>
<tr>
<th>COMP</th>
<th>F(I)</th>
<th>X(I)</th>
<th>Y(I)</th>
<th>K(I)</th>
</tr>
</thead>
<tbody>
<tr>
<td>WATER</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>MISSING</td>
</tr>
</tbody>
</table>

BLOCK: B11  MODEL: MIXER

-------------
INLET STREAMS: O2  H2
OUTLET STREAM: 14
PROPERTY OPTION SET: RKS-BM REDLICH-KWONG-SOAVE EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***
IN       OUT       RELATIVE DIFF.
TOTAL BALANCE
MOLE(KMOL/HR) 27876.3  27876.3  0.000000E+00
MASS(KG/HR ) 334800.  334800. -0.173858E-15
ENTHALPY(MMKCAL/H) 44.3476  44.3476  0.000000E+00

*** INPUT DATA ***
ONE PHASE FLASH SPECIFIED PHASE IS VAPOR
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.00010000
OUTLET PRESSURE BAR 60.0000

BLOCK: B12  MODEL: HEATX

-------------
HOT SIDE:
-------------
INLET STREAM: 14
OUTLET STREAM: 16
PROPERTY OPTION SET: RKS-BM REDLICH-KWONG-SOAVE EQUATION OF STATE
COLD SIDE:
INLET STREAM: 17
OUTLET STREAM: FEEDH2O
PROPERTY OPTION SET: RKS-BM REDLICH-KWONG-SOAVE EQUATION
OF STATE

*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th></th>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOTAL BALANCE</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MOLE(KMOL/HR)</td>
<td>46460.6</td>
<td>46460.6</td>
<td>0.000000E+00</td>
</tr>
<tr>
<td>MASS(KG/HR)</td>
<td>669600.</td>
<td>669600.</td>
<td>0.000000E+00</td>
</tr>
<tr>
<td>ENTHALPY(MMKCAL/H)</td>
<td>-1239.78</td>
<td>-1239.78</td>
<td>0.183398E-15</td>
</tr>
</tbody>
</table>

*** INPUT DATA ***

FLASH SPECS FOR HOT SIDE:
TWO PHASE FLASH
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.00010000

FLASH SPECS FOR COLD SIDE:
TWO PHASE FLASH
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.00010000

FLOW DIRECTION AND SPECIFICATION:
COUNTERCURRENT HEAT EXCHANGER
SPECIFIED HOT OUTLET TEMP
SPECIFIED VALUE C 130.0000
LMTD CORRECTION FACTOR 1.00000

PRESSURE SPECIFICATION:
HOT SIDE PRESSURE DROP BAR 0.0000
COLD SIDE OUTLET PRESSURE BAR 2.0000

HEAT TRANSFER COEFFICIENT SPECIFICATION:
HOT LIQUID COLD LIQUID KCAL/HR-SQM-K 730.8684
HOT 2-PHASE COLD LIQUID KCAL/HR-SQM-K 730.8684
HOT VAPOR COLD LIQUID KCAL/HR-SQM-K 730.8684
HOT LIQUID COLD 2-PHASE KCAL/HR-SQM-K 730.8684
HOT 2-PHASE COLD 2-PHASE KCAL/HR-SQM-K 730.8684
HOT VAPOR COLD 2-PHASE KCAL/HR-SQM-K 730.8684
HOT LIQUID COLD VAPOR KCAL/HR-SQM-K 730.8684
HOT 2-PHASE COLD VAPOR KCAL/HR-SQM-K 730.8684
HOT VAPOR COLD VAPOR KCAL/HR-SQM-K 730.8684

*** OVERALL RESULTS ***
STREAMS:

<table>
<thead>
<tr>
<th>14</th>
<th>HOT</th>
<th>16</th>
</tr>
</thead>
<tbody>
<tr>
<td>T= 2.4835D+02</td>
<td></td>
<td>T= 1.3000D+02</td>
</tr>
<tr>
<td>P= 6.0000D+01</td>
<td></td>
<td>P= 6.0000D+01</td>
</tr>
<tr>
<td>V= 1.0000D+00</td>
<td></td>
<td>V= 1.0000D+00</td>
</tr>
</tbody>
</table>

FEEDH20 └──> HOT     HOT          └──> 16
| T= 8.1616D+01 |   | T= 2.0000D+01  |
| P= 2.0000D+00 |   | P= 1.0000D+00  |
| V= 0.0000D+00 |   | V= 0.0000D+00  |

DUTY AND AREA:

CALCULATED HEAT DUTY MMKCAL/HR  23.7406
CALCULATED (REQUIRED) AREA SQM  238.1299
ACTUAL EXCHANGER AREA SQM  238.1299
PER CENT OVER-DESIGN  0.0000

HEAT TRANSFER COEFFICIENT:

AVERAGE COEFFICIENT (DIRTY) KCAL/HR-SQM-K  730.8684
UA (DIRTY) CAL/SEC-K  48344.8974

LOG-MEAN TEMPERATURE DIFFERENCE:

LMTD CORRECTION FACTOR  1.0000
LMTD (CORRECTED) C  136.4056
NUMBER OF SHELLS IN SERIES  1

PRESSURE DROP:

HOTSIDE, TOTAL BAR  0.0000
COLD SIDE, TOTAL BAR  -1.0000

PRESSURE DROP PARAMETER:

HOT SIDE:  0.00000E+00
COLD SIDE:  -8552.8

*** ZONE RESULTS ***

TEMPERATURE LEAVING EACH ZONE:

HOT

<table>
<thead>
<tr>
<th>14</th>
<th>VAP</th>
<th>16</th>
</tr>
</thead>
</table>
ZONE HEAT TRANSFER AND AREA:

ZONE HEAT DUTY AREA DTLM AVERAGE U UA
MMKCAL/HR SQM C KCAL/HR-SQM-K CAL/SEC-K
1 23.741 238.1299 136.4056 730.8684 48344.8974

BLOCK: REACTOR MODEL: HEATER

---

INLET STREAM: RIN
OUTLET STREAM: ROUT
PROPERTY OPTION SET: RKS-BM REDLICH-KWONG-SOAVE EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

IN OUT RELATIVE DIFF.
TOTAL BALANCE
MOLE(KMOL/HR) 93509.8 93509.8 0.000000E+00
MASS(KG/HR) 0.411535E+07 0.411535E+07 0.000000E+00
ENTHALPY(MMKCAL/H) -8337.02 -8135.30 -0.241960E-01

*** INPUT DATA ***

TWO PHASE PQ FLASH
SPECIFIED PRESSURE BAR 200.000
SPECIFIED HEAT DUTY MMKCAL/H 201.723
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.00010000

*** RESULTS ***

OUTLET TEMPERATURE °C 650.00
OUTLET PRESSURE BAR 200.00
OUTLET VAPOR FRACTION 1.0000
PRESSURE-DROP CORRELATION PARAMETER 0.000000E+00
V-L PHASE EQUILIBRIUM:

<table>
<thead>
<tr>
<th>COMP</th>
<th>F(I)</th>
<th>X(I)</th>
<th>Y(I)</th>
<th>K(I)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CARBO-01</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>3.8493</td>
</tr>
</tbody>
</table>
Appendix C

Listed below are the calculations performed at MIT to determine the results listed in Chapter 6. All Calculations were performed by the author using mathCAD with model data obtained from ASPEN, as shown in Appendix B.

\[ MW := 1000000 \; \text{W} \]
\[ MJ := 1000000 \; \text{J} \]
\[ r := \frac{1}{1.5397} \; \text{sec} \]

Basis: 1kg of H₂ product. Converting factor from flow rate to base:

\[ M_{\text{H}_2} := 1.5397 \; \text{kg/sec} \]
\[ M_{\text{O}_2} := 12.22 \; \text{kg/sec} \]
\[ M_{\text{CO}_2} := 203.1144 \; \text{kg/sec} \]
\[ Q_{\text{H}_2} := 33.3 \; \text{kW-hr} \]
\[ Q_{\text{Boiler}} := 32.6992 \; \text{MW} \]
\[ Q_{\text{O}_2} := 7.5075092 \; \text{MW} \]
\[ Q_{\text{ohmic}} := .991152564 \; \text{W} \]
\[ Q_{\text{preheat}} := 4.7816 \; \text{MW} \]
\[ Q_{\text{H}_2} := 15.01727 \; \text{MW} \]
\[ \eta_{\text{elec}} := .443875 \frac{600 \; \text{MW} - Q_{\text{Boiler}}}{600 \; \text{MW}} \]

Electricity produced

\[ E := 600 \; \text{MW} \cdot \eta_{\text{elec}} \]
\[ E = 45.429 \; \text{kW-hr} \]
\[ E_{\text{H}_2} := 89.3558 \; \text{MJ/kg} \]
\[ H_2 := M_{\text{H}_2} \]
\[ O_2 := M_{\text{O}_2} \]
\[ CO_2 := M_{\text{CO}_2} \]
\[ \text{Duty}_{\text{preheat}} := Q_{\text{preheat}} \]
\[ \text{Duty}_{\text{Boiler}} := Q_{\text{Boiler}} \]
\[ \text{Duty}_{\text{ohmic}} := Q_{\text{ohmic}} \]
\[ \text{Duty}_{O_2} := Q_{O_2} \]
\[ \text{Duty}_{H_2} := Q_{H_2} \]
\[ \text{Duty}_{\text{water}} := \text{Duty}_{\text{Boiler}} + \text{Duty}_{\text{ohmic}} + \text{Duty}_{O_2} + \text{Duty}_{H_2} + \text{Duty}_{\text{preheat}} \]
Properties of HTSE plant 1 MPa:

1. kWhr of electrical energy:
   produced in reactor
   \[ E = 45.429 \text{kW-hr} \]
   required for 1 kg of H2 product
   \[ H_2 \cdot E_{H_2} = 24.821 \text{kW-hr} \]
   required for ohmic heating
   \[ \text{Duty}_{\text{ohmic}} = 0.179 \text{kW-hr} \]
   remaining for the grid
   \[ E - E_{H_2} - H_2 - \text{Duty}_{\text{ohmic}} = 20.429 \text{kW-hr} \]

2. kWhr recuperated from:
   H2 product
   \[ \text{Duty}_{H_2} = 2.709 \text{kW-hr} \]
   O2 product
   \[ \text{Duty}_{O_2} = 1.354 \text{kW-hr} \]

3. kWhr required for water boiler:
   \[ \text{Duty}_{\text{Boiler}} = 5.899 \text{kW-hr} \]

4. kWhr needed to heat steam:
   \[ \frac{1.79}{11.044} = 0.016 \]
   to operating temperature:
   \[ \text{Duty}_{\text{water}} = 11.004 \text{kW-hr} \]
   \[ \text{Duty}_{\text{ohmic}} = 0.179 \text{kW-hr} \]
   (Energy required in ohmic heater is less than 1.6% of total energy required.)

Electrical Efficiency: 41.97%
Dostal's efficiency: 44.39%

If design is adjusted for 6 MPa production:

\[ r := \frac{1}{1.5274} \sec \]

Basis: 1kg of H2 product. Converting factor from flow rate to base:

\[ M_{H_2} := 1.5274 \frac{\text{kg}}{\sec} \]
\[ M_{O_2} := 12.22 \frac{\text{kg}}{\sec} \]
\[ M_{CO_2} := 203.1144 \frac{\text{kg}}{\sec} \]
\[ Q_{\text{Boiler}} := 32.699 \text{MW} \]
\[ Q_{O_2} := 8.08059216 \text{MW} \]
\[ Q_{\text{ohmic}} := 1.013874 \text{MW} \]
\[ Q_{\text{H}_2} := 14.039835 \text{MW} \]
\[ \eta_{\text{elec}} := \frac{600 \text{MW} - Q_{\text{Boiler}}}{600 \text{MW}} \]
\[ Q_{\text{preheat}} := 4.7810 \text{MW} \]

Electricity produced

\[ E_{\text{H}_2} := 89.3558 \text{MJ/kg} \]
\[ E := 600 \text{MW} \cdot \eta_{\text{elec}} \]
\[ E = 45.795 \text{kW·hr} \]
\[ H_2 := M_{\text{H}_2} \]
\[ O_2 := M_{\text{O}_2} \]
\[ CO_2 := M_{\text{CO}_2} \]
\[ \text{Duty}_{\text{preheat}} := Q_{\text{preheat}} \]
\[ \text{Duty}_{\text{Boiler}} := Q_{\text{Boiler}} \]
\[ \text{Duty}_{\text{ohmic}} := Q_{\text{ohmic}} \]
\[ \text{Duty}_{O_2} := Q_{O_2} \]
\[ \text{Duty}_{H_2} := Q_{H_2} \]
\[ \text{Duty}_{\text{water}} := \text{Duty}_{\text{Boiler}} + \text{Duty}_{\text{ohmic}} + \text{Duty}_{O_2} + \text{Duty}_{H_2} + \text{Duty}_{\text{preheat}} \]

**Properties of Revised HTSE plant:**

1. kWhr of electrical energy:
   produced in reactor
   \[ E = 45.795 \text{kW·hr} \]
   required for 1 kg of H2 product
   \[ H_2 E_{\text{H}_2} = 24.821 \text{kW·hr} \]
   required for ohmic heating
   \[ \text{Duty}_{\text{ohmic}} = 0.184 \text{kW·hr} \]
   remaining for the grid
   \[ E - H_2 E_{\text{H}_2} - \text{Duty}_{\text{ohmic}} = 20.79 \text{kW·hr} \]

2. kWhr recuperated from:
   H2 product
   \[ \text{Duty}_{H_2} = 2.553 \text{kW·hr} \]
   O2 product
   \[ \text{Duty}_{O_2} = 1.47 \text{kW·hr} \]

3. kWhr required for water boiler:
   \[ \text{Duty}_{\text{Boiler}} = 5.947 \text{kW·hr} \]

4. kWhr needed to heat steam:
   to operating temperature:
Duty\textsubscript{water} = 11.024\text{KWh}\
Duty\textsubscript{ohmic} = 0.184\text{KWh}\
\frac{Duty\textsubscript{ohmic}}{Duty\textsubscript{water}} = 0.0167

Energy for Ohmic heating is 1.7\% of total
Electrical Efficiency: 41.97\%
Dostal's efficiency: 44.39\%

**Steam Turbine Design:**

\[ r := \frac{1}{1.5274} \text{ sec} \]

Basis: 1\text{kg} of H\textsubscript{2} product. Converting factor from flow rate to base:

\[ M\textsubscript{H2} := 1.5274\text{kg/sec} \]
\[ M\textsubscript{H2O} := 12.7\text{kg/sec} \]
\[ Q\textsubscript{O2} := 7.009521\text{MW} \]
\[ Q\textsubscript{Boiler} := 32.6993\text{MW} \]
\[ Q\textsubscript{ohmic} := 1.0138739\text{MW} \]
\[ Q\textsubscript{turbine} := 0.5169069\text{MW} \]
\[ Q\textsubscript{H2} := 12.178875\text{MW} \]
\[ \eta\textsubscript{elec} := 0.443875 \frac{600\text{MW} - Q\textsubscript{Boiler}}{600\text{MW}} \]
\[ Q\textsubscript{preheat} := 6.113\text{MW} \]

Electricity produced

\[ E\textsubscript{H2} := 89.3558\text{MJ/kg} \]
\[ E := 600\text{MW} \cdot \eta\textsubscript{elec}^{-1} \]
\[ E = 45.795\text{KWh} \]
\[ H\textsubscript{2} := M\textsubscript{H2}^{-1} \]
\[ O\textsubscript{2} := M\textsubscript{O2}^{-1} \]
\[ H20 := M\textsubscript{H2O}^{-1} \]
\[ \text{Duty\textsubscript{preheat}} := Q\textsubscript{preheat}^{-1} \]
\[ \text{Duty\textsubscript{Boiler}} := Q\textsubscript{Boiler}^{-1} \]
\[ \text{Duty\textsubscript{ohmic}} := Q\textsubscript{ohmic}^{-1} \]
\[ \text{Duty\textsubscript{O2}} := Q\textsubscript{O2}^{-1} \]
\[ \text{Duty\textsubscript{H2}} := Q\textsubscript{H2}^{-1} \]
\[ \text{Duty\textsubscript{water}} := \text{Duty\textsubscript{Boiler}} + \text{Duty\textsubscript{ohmic}} + \text{Duty\textsubscript{O2}} + \text{Duty\textsubscript{H2}} + \text{Duty\textsubscript{preheat}} \]
\[ \text{Duty\textsubscript{Turbine}} := Q\textsubscript{turbine}^{-1} \]
Properties of Revised HTSE plant:

1. kWhr of electrical energy:
   produced in reactor
   \[ E = 45.795 \text{kW-hr} \]
   required for 1 kg of H2 product
   \[ H_2 \cdot E_{H_2} = 24.821 \text{kW-hr} \]
   required for ohmic heating
   \[ \text{Duty}_{\text{ohmic}} = 0.184 \text{kW-hr} \]
   remaining for the grid
   \[ E - E_{H_2} \cdot H_2 - \text{Duty}_{\text{ohmic}} = 20.79 \text{kW-hr} \]

2. kWhr recuperated from:
   \[ \text{H}_2 \text{ product} \]
   \[ \text{Duty}_{H_2} = 2.215 \text{kW-hr} \]
   \[ \text{O}_2 \text{ product} \]
   \[ \text{Duty}_{O_2} = 1.275 \text{kW-hr} \]

3. kWhr required for water boiler:
   \[ \text{Duty}_{\text{Boiler}} = 5.947 \text{kW-hr} \]

4. kWhr needed to heat steam:
   to operating temperature:
   \[ \text{Duty}_{\text{water}} = 10.733 \text{kW-hr} \]
   \[ \text{Duty}_{\text{ohmic}} = 0.184 \text{kW-hr} \]
   \[ \frac{\text{Duty}_{\text{ohmic}}}{\text{Duty}_{\text{water}}} = 0.017 \]
   Energy for Ohmic heating is 1.7% of total
   Electrical Efficiency: 41.97%
   Dostal's efficiency: 44.39%

5. Energy Extracted from Turbine:
   \[ \text{Duty}_{\text{Turbine}} = 0.094 \text{kW-hr} \]
   \[ \text{MW} := 1000000 \text{W} \]
   \[ \text{MJ} := 1000000 \text{J} \]

Basis: 1 kg of H2 product. Converting factor from flow rate to base:

\[ M_{H_2} := 10.4065458 \frac{\text{kg}}{\text{sec}} \]

\[ r := \frac{\text{kg}}{M_{H_2}} \]

\[ M_{O_2} := 82.59 \frac{\text{kg}}{\text{sec}} \]

\[ M_{CO_2} := 1143.152 \frac{\text{kg}}{\text{sec}} \]

\[ Q_T := 11.91 \text{MW} \]

\[ Q_{\text{Boiler}} := 234.6 \text{MW} \]

\[ Q_{O_2} := 57.6463042 \text{MW} \]
\[ P_{th} := 2550 \text{MW} \]
\[ Q_{\text{ohmic}} := 6.9077125 \text{MW} \]
\[ Q_{\text{preheat}} := 27.4749 \text{MW} \]
\[ Q_{\text{H}_2} := 100.159 \text{MW} \]

\[ \eta_{\text{elec}} := \frac{.468516}{\left( \frac{P_{th} - Q_{\text{Boiler}}}{P_{th}} \right)} \]

Electricity produced
\[ E := P_{th} \eta_{\text{elec}} \]
\[ E = 28.956 \text{kW-hr} \]

\[ E_{\text{H}_2} := 89.35581.1 \text{MJ} \]

Duty \( T \) := \( Q_{T} \)
\[ \text{H}_2 := M_{\text{H}_2} \]
\[ O_{2} := M_{O_{2}} \]
\[ \text{CO}_2 := M_{\text{CO}_2} \]

Duty_{\text{preheat}} := \( Q_{\text{preheat}} \)

Duty_{\text{Boiler}} := \( Q_{\text{Boiler}} \)

Duty_{\text{ohmic}} := \( Q_{\text{ohmic}} \)

Duty_{O_{2}} := \( Q_{O_{2}} \)

Duty_{\text{H}_2} := \( Q_{\text{H}_2} \)

Duty_{\text{water}} := Duty_{\text{Boiler}} + Duty_{\text{ohmic}} + Duty_{O_{2}} + Duty_{\text{H}_2} + Duty_{\text{preheat}}

\textbf{Properties of HTSE at 10 \% overpotential:}

\[ \frac{E}{.4054} = 71.426 \text{kW-hr} \]

1. kWhr of electrical energy:
   produced in reactor
   \[ \frac{E}{.4054 - 3.18 \times 10^{-4}} = 2271.4 \text{MW} \]
   \[ E = 28.956 \text{kW-hr} \]
   required for 1 kg of H2 product
   \[ \eta_{\text{elec}} = 0.425 \]
   \[ H_{2}E_{\text{H}_2} = 27.303 \text{kW-hr} \]
   \[ \frac{.318 \cdot 1083}{28.956} = 2.973 \]
   required for ohmic heating
   \[ \frac{2274}{.89} = 2.555 \times 10^{3} \]
   \[ \text{Duty}_{\text{ohmic}} = 0.184 \text{kW-hr} \]
remaining for the grid
\[ \frac{2274 \times 10^3}{85} = 1.253 \times 10^3 \]
\[ E = E_H^2 - H_2 - \text{Duty}_{\text{ohmic}} = 1.469\text{MW} \cdot \text{hr} \]

2. kWh recuperated from:
\[ P_{\text{req}} = 71.496 \frac{\text{kW} \cdot \text{hr}}{\text{kg}} - 3.18 \times 10^4 \frac{\text{kg}}{\text{hr}} \]

H2 product
\[ \text{Duty}_{H_2} = 2.674\text{MW} \cdot \text{hr} \]
\[ P_{\text{req}} = 2.274 \times 10^3 \text{MW} \]

O2 product
\[ P_{\text{req}} = 0.892 \frac{\text{MW}}{2550} \]
\[ \text{Duty}_{O_2} = 1.539\text{MW} \cdot \text{hr} \]

3. kWh required for water boiler:
\[ 2700.85 = 2.295 \times 10^3 \]
\[ \text{Duty}_{\text{Boiler}} = 6.262\text{MW} \cdot \text{hr} \]

4. kWh needed to heat steam:
\[ \frac{11.044}{11.79} = 0.016 \]

5. Steam Turbine Work Derived
\[ \text{Duty}_T = 0.318\text{MW} \cdot \text{hr} \]
\[ \frac{6.262 \times 2550}{71.496} = 55.836 \]
\[ \eta_{H_2} = \frac{C_{H_2}}{\text{Duty}_{\text{Boiler}} + \frac{H_2 \cdot E_{H_2}}{\eta_{\text{elec}}}} \]
\[ \eta_{H_2} = 0.473 \]

Basis: 1 kg of H2 product. Converting factor from flow rate to base:
\[ M_{H_2} : = 93 \frac{\text{kg}}{\text{sec}} \]
\[ r : = \frac{\text{kg}}{M_{H_2}} \]
\[ M_{O_2} : = 22.5578 \frac{\text{kg}}{\text{sec}} \]
\[ M_{CO2} := 1143.152 \frac{kg}{sec} \]
\[ Q_T := 7.985 MW \]
\[ Q_{Boiler} := 234.6 MW \]
\[ Q_{O2} := 24.460380 MW \]
\[ Q_{ohmic} := 3.288591 MW \]
\[ Q_{H2} := 42.4993 MW \]
\[ (1200 \times 120 MW - Q_{Boiler} : 1 \text{lelec} := 0.468516 \times 0.9 \times 120 MW - Q_{Boiler} \times 0.9 \]
\[ Q_{preheat} := 21.2476547 MW \]
\[ \text{Electricity produced} \]
\[ E := 1200 \times \eta_{elec} \times 1 \text{lelec} \]
\[ E = 1.324 \text{kW} \cdot \text{hr} \]
\[ E_{H2} := 89.35581.1 \frac{MJ}{kg} \]
\[ \text{Duty}_{T} := Q_T \times 1 \]
\[ H_2 := M_{H2} \]
\[ O_2 := M_{O2} \]
\[ CO2 := M_{CO2} \]
\[ \text{Duty}_{preheat} := Q_{preheat} \times 1 \]
\[ \text{Duty}_{Boiler} := Q_{Boiler} \times 1 \]
\[ \text{Duty}_{ohmic} := Q_{ohmic} \times 1 \]
\[ \text{Duty}_{O2} := Q_{O2} \times 1 \]
\[ \text{Duty}_{H2} := Q_{H2} \times 1 \]
\[ \text{Duty}_{water} := \text{Duty}_{Boiler} + \text{Duty}_{ohmic} + \text{Duty}_{O2} + \text{Duty}_{H2} + \text{Duty}_{preheat} \]

**Properties of HTSE at 10 % overpotential with generator \( \eta \) (-2%):**

1. **kWhr of electrical energy:**
   produced in reactor
   \[
   \frac{E}{\eta_{elec}} \times 3.18 \times 10^4 \frac{1}{hr} = 113.978 MW
   \]
   \[ E = 1.324 \text{kW} \cdot \text{hr} \]
   required for 1 kg of H2 product
   \[ H_2 \cdot E_{H2} = 27.303 \text{kW-hr} \]
   required for ohmic heating
   \[ \text{Duty}_{ohmic} = 9.823 \times 10^{-3} \text{ kW} \cdot \text{hr} \]
   \[ \frac{28.528}{.424} = 67.283 \]
remaining for the grid
\[ \frac{27.182}{0.404} = 67.282 \]
\[ E - E_{H2} \cdot H2 - \text{Duty}_{ohmic} = -25.989 \text{ kW} \cdot \text{hr} \]
2. kWhr recuperated from:
\[ 1 \frac{\text{lb}}{\text{day} \cdot \text{hr}} = 0.019 \frac{\text{kg}}{\text{hr}} \]
H2 product
\[ \text{Duty}_{H2} = 0.127 \text{ kW} \cdot \text{hr} \]
O2 product
\[ \text{Duty}_{O2} = 0.073 \text{ kW} \cdot \text{hr} \]
3. kWhr required for water boiler:
\[ \text{Duty}_{\text{Boiler}} = 0.701 \text{ kW} \cdot \text{hr} \]
4. kWhr needed to heat steam:
\[ \frac{.179}{11.044} = 0.016 \]
to operating temperature:
\[ \text{Duty}_{\text{water}} = 0.974 \text{ kW} \cdot \text{hr} \]
\[ \text{Duty}_{\text{ohmic}} = 9.823 \times 10^{-3} \text{ kW} \cdot \text{hr} \]
(Energy required in ohmic heater is less than 1.6% of total energy required.)
Net Efficiency: 41.79%
Dostal's efficiency: 41.97%
5. Steam Turbine Work Derived
\[ \eta_{\text{elec}} = 0.369 \]
\[ \text{Duty}_{T} = 0.024 \text{ kW} \cdot \text{hr} \]
\[ \eta_{H2} = \frac{G_{H2}}{\text{Duty}_{\text{Boiler}} + \frac{E_{H2}}{\eta_{\text{elec}}}} \]
\[ \eta_{H2} = 0.446 \]
\[ r := \frac{1}{5.5949} \text{ sec} \]
Basis: 1 kg of H2 product. Converting factor from flow rate to base:
\[ M_{\text{CO2}} := 645.0897 \frac{\text{kg}}{\text{sec}} \]
\[ M_{\text{H2O}} := 50 \frac{\text{kg}}{\text{s}} \]
\[ M_{H2} := 5.5949 \frac{\text{kg}}{\text{sec}} \]
\[ Q_T := 9.928860 \text{ MW} \]
\[ Q_{\text{Boiler}} := 129.6 \text{ MW} \]
\[ Q_{O2} := 26.400484 \text{ MW} \]
\[ Q_{\text{ohmic}} := 3.7138239 \text{ MW} \]

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\[ Q_{\text{preheat}} = 27.3423619 \text{MW} \]
\[ Q_{\text{H2}} = 45.8702093 \text{MW} \]

\[ \eta_{\text{elec}} = 0.468516 \left( \frac{1200 \text{MW} - Q_{\text{Boiler}}}{1200 \text{MW}} \right) \]

Electricity produced

\[ E = 1200 \text{MW} \cdot \eta_{\text{elec}} \]
\[ E = 24.899 \text{kW} \cdot \text{hr} \]
\[ E_{\text{H2}} = 89.3558 \text{MJ} \]
\[ \text{Duty}_T = Q_{\text{T}} \]
\[ \text{H}_2 = M_{\text{H2}} \]
\[ \text{O}_2 = M_{\text{O2}} \]
\[ \text{CO}_2 = M_{\text{CO2}} \]
\[ \text{Duty}_{\text{preheat}} = Q_{\text{preheat}} \]
\[ \text{Duty}_{\text{Boiler}} = Q_{\text{Boiler}} \]
\[ \text{Duty}_{\text{ohmic}} = Q_{\text{ohmic}} \]
\[ \text{Duty}_{\text{O2}} = Q_{\text{O2}} \]
\[ \text{Duty}_{\text{H2}} = Q_{\text{H2}} \]
\[ \text{Duty}_{\text{water}} = \text{Duty}_{\text{Boiler}} + \text{Duty}_{\text{ohmic}} + \text{Duty}_{\text{O2}} + \text{Duty}_{\text{H2}} + \text{Duty}_{\text{preheat}} \]

Properties of HTSE at 0 % overpotential:

1. kWhr of electrical energy:
   produced in reactor
   \[ E = 24.899 \text{kW} \cdot \text{hr} \]
   required for 1 kg of H2 product
   \[ H_2 \cdot E_{\text{H2}} = 24.821 \text{kW} \cdot \text{hr} \]
   required for ohmic heating
   \[ \text{Duty}_{\text{ohmic}} = 0.184 \text{kW} \cdot \text{hr} \]
   remaining for the grid
   \[ E - H_2 \cdot E_{\text{H2}} - \text{Duty}_{\text{ohmic}} = -0.107 \text{kW} \cdot \text{hr} \]

2. kWhr recuperated from:
   H2 product
   \[ \text{Duty}_{\text{H2}} = 2.277 \text{kW} \cdot \text{hr} \]
   O2 product
   \[ \text{Duty}_{\text{O2}} = 1.311 \text{kW} \cdot \text{hr} \]

3. kWhr required for water boiler:
   \[ \text{Duty}_{\text{Boiler}} = 6.434 \text{kW} \cdot \text{hr} \]

4. kWhr needed to heat steam:
to operating temperature:
Duty_{water} = 11.564\text{ kW-hr}
Duty_{ohmic} = 0.184\text{ kW-hr}

(Energy required in ohmic heater is less than 1.6\% of total energy required.)
Electrical Efficiency: 41.79\%
Dostal's efficiency: 41.97\%

5. Steam Turbine Work Derived
Duty_T = 0.493\text{ kW-hr}

\[ M := \frac{1 \text{ kg}}{1000 \text{ mol}} \]
\[ R_g := 0.0821 \frac{\text{ atm-L}}{\text{ mol-K}} \]
\[ T := 303.1^\circ \text{K} \]
\[ P \cdot V = n \cdot R \cdot T \]
\[ \frac{n}{V} = \frac{P}{R \cdot T} \]

\[ \eta_{H_2} := \frac{G_{H_2}}{\text{Duty_{Boiler} + H_2} \cdot \frac{F_{H_2}}{\eta_{elec}}} \]
\[ Q := 300 \times 10^6 \frac{\text{ ft}^3}{\text{ day}} \]
\[ \rho := 56 \times 10^{-4} \frac{\text{ lb}}{\text{ ft}^3} \]
\[ \rho \cdot Q = 3.175 \times 10^4 \frac{\text{ kg}}{\text{ hr}} \]
\[ \eta_{H_2} = 0.506 \]