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Hydrogen Generation using Solar Reactor

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Contents

1	Contribution of Abrar Sobhan Chowdhury	3
2	Contribution of Md Sadatuzzaman Saagoto	6
3	Contribution of Junayed Bin Zakir	8
4	Abstract	10
5	Introduction	10
6	System Description	13
7	Equations	16
8	Results and Discussion	18
9	Conclusion	24
10	Appendix	25
11	References	30

1 Contribution of Abrar Sobhan Chowdhury

In the "Applied Thermodynamics Lab" Project, initially I took the initiative to form a team. After team formation, we shortlisted three topics to work on and finally through a group meeting we decided to work on "Hydrogen Generation using Solar Energy" since we were interested in renewables. Later, we collected papers from renowned journals on the mentioned topic. We went through 7 or 8 papers in order to decide which one to follow. We were confused between two paper of which one was "Thermodynamic analysis of a solar-driven high-temperature steam electrolyzer for clean hydrogen production" by Wei et al. published in "Applied Thermal Engineering" journal of Elsevier. After a group discussion regarding the papers, we agreed upon choosing "Energy and exergy analyses of an integrated renewable energy system for hydrogen production" by Ali M.M.I. Qureshy and Ibrahim Dincer published in "Energy" journal of Elsevier.

We have decided to go through the paper thoroughly in order to have a concrete idea about the things we will be doing. Since this project's goal is to validate the chosen paper, it was essential for each one of us to understand the concepts of the paper. The paper introduced me with a new theoretical system developed by the authors to generate hydrogen using solar energy. Since, I personally didn't have much idea regarding the whole process of hydrogen generation, I had to watch a few YouTube videos and had to read a few articles on hydrogen generation using solar energy and it's current progress to get a good grasp on the topic. The paper mentioned several works of the hydrogen generation systems developed previously by researchers along with their obtained efficiencies. Apart from that, the concepts of entropy and exergy were also needed to be brushed up.

We have understood the working procedure of the integrated system developed in the paper and analysed the equation as well as the results obtained from the system. After a group discussion, we divided the work and I started working on the coding section. Initially, I have tried to work with CoolProp in both Python and Matlab. But, things didnt work out as expected. After spending a decent amount of time on trying to install Coolprop in both Python and Matlab but failing every time, eventually I gave up. And since this paper used EES (Engineering Equation Solver) code to solve the simultaneous equations, I started learning EES watching YouTube videos. Moreover,

along with my teammate Saagoto, we have worked together in order to grasp the whole concept of writing a code in EES.

I, myself wrote a code in EES to calculate the the results and validate the values from the paper. As the equations pertaining to each component was provided in the paper, I have used those equations accordingly to solve the system output. Moreover, in the paper, mass flow rate, enthalpy, entropy, temperature, pressure and specific exergy of the specific states in the system was tabulated. Using those tabulated values as initial state points, I've solved the mentioned equations. The results obtained from EES had some discrepancies in some of the components. I discussed the issue with my teammate, who solved the code separately, also had the same problem. Afterwards, we figured out some of the assumptions and results obtained from the paper was not correct. Some values were also missing which we've used from searching the internet.

We have emailed the authors of the paper regarding the issue we faced mentioning the problems specifically. Unfortunately, we still didn't get any response from them.

Though most of the results from the paper were validated from the EES code, yet some values couldn't be validated. Discrepancies in solar reactor and liquidification caused the results to deviate from our obtained results.

Since, we had confusion regarding some of the values mentioned in the paper and the results obtained by them, we even wrote an EES code using the exact same values from the paper and it was found that the calculated efficiency of the paper and EES code was different though it should have been same.

Apart from the EES code, I was involved in making the PowerPoint presentation for the consultation rounds along with my teammates through a group discussion. We had group meeting almost every week to discuss our work progress and what to do next and how to proceed further.

Lastly, we came to conclusion that, there might be some mistake in the paper and, proceeded with our final report. The final report was intructed to be compiled in Latex. I had some experience on using Latex previously, so I helped my teammates especially Junayed as he was mainly compiling the report, to write the report as well as tried to help them in solving problems they faced. I have compiled the equations portion and state points in Latex for the final report.

I have learnt quite a few things doing this project and have spent more than 45 hours in completing this project successfully. I believe my teammates and I have equal contribution in the success of this project which wouldn't be possible without their cooperation.

2 Contribution of Md Sadatuzzaman Saagoto

At the very beginning of the lab, I had gone through seven or eight papers, and then after meeting with the teammates, we selected the paper. I spent several hours grasping the paper and the system proposed in that. As the paper was related to energy and exergy analysis, it was needed to go through energy, entropy, and exergy concepts. It took a fair amount of time. After that, I was trying to learn a programming language to model the system mathematically. First, I tried with python and set up “CoolProp”. I had learnt few basics, but it was entirely new for me. I did not feel confident and tried “CoolProp” in MATLAB. MATLAB was familiar to me as I had some previous coding experience in MATLAB. However, when I saw the modelling of the system was done in EES in the paper, I just tried to recreate it. EES seemed interesting because I have seen many problems in our textbook, which were advised to solve with EES. My journey with EES begun.

I faced some problems while downloading the software because neither it was free nor open-source software. I downloaded a crack version, but it did not work. After searching for a while, I got a licence which was shared in the “ResearchGate.” From the link given there, I downloaded EES. After setting it up on my PC, I started learning it. Learning the nomenclature and syntax did not take much time. I went through some of the YouTube videos and official EES documentation and then tried to solve mathematical problems given in our book in EES.

I wrote nearly 170 equations in EES, and keeping track of all these equations was not easy. In EES h_1 , $h1$, $h[1]$, all these three will give output $h1$, but they are not the same. I learnt this while I was working with the property plot. I think the plotting options in EES are the most convenient than using python or MATLAB for thermodynamic property plots. For plotting in EES, no coding is required; with a few clicks, graphs can be plotted. I plotted all the graphs in our work and wrote all the equations except the equations of exergy. I plotted the bar and pie charts using Excel. It was much more convenient. After plotting, the most helpful feature of EES is the option for creating parametric tables. It took only a minute or two to complete some of the parametric study done in the paper. Finding thermodynamic property values at different points is also very easy using the ‘Function’ option. EES coding was comfortable for me because it took less coding with more clicking

in different options. Also, the coding is not like coding in ‘C’. It’s more like the English language and very easy to understand.

After completing the coding part, I helped my teammates in writing. We divided the writings into several parts, and each part was assigned to us. I wrote my part in ‘Word’ and forwarded it. One of our teammates compiled the writings and coded them in latex.

We equally contributed to the bi-weekly presentation preparation and progress report. I am thankful to my teammates, as they helped me a lot. They were cooperative and never complained if something was not going smoothly. Every week, we sat for a virtual meeting at least once from the very beginning of the project. Our team put a great effort to make this a successful project. It was an extraordinary journey to be a part of the team and recreating the paper.

3 Contribution of Junayed Bin Zakir

Initially when starting this project for 'Applied thermodynamics Lab' I had assisted my teammates in going through a collection of papers so that we may choose a suitable paper to use for our project. We had discussed several papers and their methodologies in depth and finally decided on one to replicate. Due to the relatively complex nature of the concepts and calculations used in the paper that we had selected it took some time to comprehend all the concepts and to understand how to suitably use all the equations. As we were planning on replicating the paper and its methodology some time was needed to fully grasp all the components of the system and how they interacted as well.

Primarily, my personal contribution to the paper is the understanding of LATEX and how to use it to compile the disparate elements of our findings and present it as a report. In order to do this I first spent some days watching tutorials on how to use LATEX to understand how the format functioned and how to best use it.

Initially I had attempted to use a TEX editor on my computer using MiKTeX but ran into a host of issues trying to use it on my PC. As a result I opted to look for alternatives. Eventually I settled on using 'Overleaf' which is an online Tex editor and compiler. I used the site to create the report that is currently being read.

Over the time I spent on this reports I had to learn many elements of LATEX programming including the inclusion of images, tables, equations and references. I had to spend some time on learning how to insert these elements and edit their formatting and presentation so as to make it consistent with the rest of the report.

Furthermore, I was the one responsible for most of the text of the report itself. I had thoroughly gone through the paper that we had used as a reference for this report and used it as a template to write our own, taking care to not make the two papers overly similar.

The analysis and presentation of the obtained results was a collaborative effort from our team. We discussed the results and created points on the disparities and I was the one responsible for writing it out in prose and making it presentable. With the help of my teammates I had also learnt a great deal about EES and how the equation formatting for the software

works.

Overall I believe I have spent upwards of 35 hours on this report. Most of the knowledge I have gained is related to LATEX programming, but I have learned a good deal about EES programming and simulation as well. My teammates contribution to this project was substantial and the compilation and presentation of this report would not have been possible without considerable collaboration from everyone involved. I believe that we all helped each other immensely and our combined efforts and ready co-operation was what made this report possible.

4 Abstract

This paper showcases our attempt to replicate the energy and exergy efficiency result of a proposed solar driven, high temperature steam electrolyzer. We use a given paper as a reference for our work. We use EES to process the given equations and compare results to the reference. We find some disparities and discuss them in the report. Our methodology is given here for review as well. This was done in the hopes of showcasing the feasibility of using renewable energy sources as a method of electricity generation. We have included a schematic of the system used as well as the code we used in EES. Our results are given in both graphical and tabular format.

5 Introduction

The ability to produce sustainable renewable energy is one of the major issues currently plaguing the globe. It is estimated that by the year 2050 upwards of 50 TW of energy may be necessary to accommodate the globe's ever increasing population as well as the inflation of the economy. Due to their significant negative impact on the environment and their unsustainability it was decided that fossil fuels would have to be phased out of use by the year 2030 [RML08]. Out of all other options, Hydrogen is currently considered one of the more favorable replacements for fossil fuels due to its abundant and clean nature [Jai09]. Moreover, hydrogen as an energy source has other positive aspects including flexibility of use and ease of storage. Being said, at present fossil fuels make up 95 percent of all the resources currently in use for the production of hydrogen [HW15]. Though many other means are employed as well for hydrogen production, including: solar, wind, geothermal, hydro-power, geothermal etc [DA15a]. Due to necessity, special attention has been given by researchers to the methods of hydrogen production that utilize renewable sources of energy. Of course, this was done due to increase sustainability of said forms of production so that they could feasibly replace fossil fuels [DA15b].

There are a number of ways to generate hydrogen. They are:

1. Photo-electical water splitting [AD18] [MDA18] [MDB10].
2. Thermochemical water decomposition [MDA17] [ARo09].
3. Water splitting via solar electricity [MM18] [MAA+19] [EK10].

To ensure that we use the most suitable production technique for a given application, we should conduct an analysis that takes many factors into account. Factors such as the cost, the availability of the energy source and the environmental impact all must be taken into consideration. Maximizing the rate of production of hydrogen whilst minimizing the costs remain the most prioritized of all the factors. Many parameters are looked at when conducting an analysis of such a system, the physical analysis consisting of the electrode material composition, electrolyte composition, photovoltaic cells and the design of the reactor itself. A thermodynamic analysis of the system is what we are going to be conducting in order to determine the efficiency.

We have examined a number of papers in order to design the system that we will analyze in this paper. One important paper was written by one Stuart Licht [[Lic05](#)]. He carried out an examination of various techniques of experimental hydrogen production. Those techniques included direct, indirect and hybrid thermochemical routes. He reported that through reaching a specific set of conditions by carefully regulating the insulation, temperature, pressure and the photosensitizer bandgap it was possible to reach an efficiency of 50 percent when it comes to solar to hydrogen conversion.

The thermodynamic analysis procedures that we are employing in this paper were largely taken from a paper by Ali M.M.I Qureshi and Ibrahim Dincer [[MD20](#)]. The purpose of that particular paper was to carry out the energy and exergy analysis of multiple integrated renewable energy systems for hydrogen production. For this paper, our approach to Thermodynamic analysis will be mirroring the aforementioned paper. Similarly our analysis will also be conducted using EES (Engineering Equation Solver). The conditions for EES are specified and the mass, entropy, energy, and exergy balance equations that will be used for each component that constitute the system will be provided.

The system that we are going to be using is a solar driven, high temperature steam electrolyzer. We will construct a conceptual design and use a real-time simulator to conduct a thermodynamic analysis. In order to provide the electrolyzer with sufficient power we are going to be using a solar-driven Rankine cycle. The Rankine cycle is a thermodynamic cycle that is primarily used to model the processes through which thermal energy is converted to mechanical work. Therefore it is ideal for the system that we have created. In order to provide the necessary power to run the cycle we are going to be

using the oil flow between a supplier and a storage tank. Finally the system utilizes a high performance electrolyzer with a hydrogen separation efficiency of 98 percent.

For us the purpose of this paper is to carry out an attempt at replicating and thus verifying the contents of the paper that we are using as a reference. From this we hope that we can demonstrate the validity of utilizing such a system as an alternative means of producing energy. As mentioned before the ever approaching dearth of natural resources that the planet is headed for due to our reliance on said resource is a problem that should be given the upmost of prioritization and consideration and in our opinion we as a society should be taking preemptive measures to ensure that a lack of resources to the extent of causing cataclysmic societal discord is never experienced. In order to further this, in our opinion, justified end we have resolved to demonstrate the feasibility of systems that primarily run on renewable energy sources in order to hopefully sway the scientific consensus on how realistic it is to expect such a thing.

Each of the devices that make up the system will be analyzed using the 1st and the 2nd Law of Thermodynamics. The individual constituents of the devices will be taken as control volumes for the purpose of analysis. We have made a number of assumptions regarding the system for this paper. They are:

1. We assumed that all of the devices that make up the system experience Steady State Steady Flow.
2. The loss of pressure caused by the connecting pipes is assumed to be negligible.
3. We considered the outlet temperature of the boiler to be constant and assumed that it is equal to the maximum temperature of the Rankine cycle.
4. The storage tank was designed in a way to ensure the temperature is set at a fixed value above the maximum temperature of the Rankine cycle in order to operate the system.
5. The ambient temperature and pressure are considered to be 298 K and 101.3 kPa respectively for our simulation.
6. We assumed that the Generator and isentropic efficiencies of the turbine are 80 percent and 90 percent respectively.
7. It was assumed that the motor and isentropic efficiencies of compressor are 80 percent and 85 percent respectively.

8. We assumed that motor and isentropic efficiencies of the pumps are 95 percent and 85 percent respectively.

9. We proceeded under the assumption that the heat and pressure losses in the turbines, compressors, pumps, and the pipelines are negligible.

With this paper, what we hope to accomplish is the design of a system and its corresponding thermodynamic model in accordance with the mentioned reference paper. Through the use of the simulation we hope to demonstrate that the system exhibits a high degree of efficiency in regard to its ability to separate pure hydrogen from the feed water.

6 System Description

The system we have considered is the same as mentioned in [\[MD20\]](#).

At point 1, the makeup water enters pump two and circulates through the heat exchanger, where the water gets pre-heated and goes to the solar receiver. The solar receiver receives heat from the solar radiation reflected by the heliostats. The pre-heated water converts to the superheated steam at the outlet of the solar receiver. The superheated steam gets divided into two parts; a portion goes to the solar reactor and another to the high-pressure turbine. The solar reactor also receives heat from solar radiation reflected by the heliostats. The solar reactor produces hydrogen and oxygen from the superheated steam. After receiving steam from the solar receiver, the high-pressure turbine gives the output to the medium-pressure turbine. The fluid leaving from the HPT goes to the solar receiver again. The output shaft of the MPT connects it to the condensing turbine. The fluid leaving from MPT goes to the heat exchanger and loses its heat to the incoming water stream from the second pump. After losing heat, it goes through the condensing turbine. The CT runs the electric generator, and leaving fluid goes through the intercooler and cools down, and the first pump increases the pressure of the water.

The output hydrogen is then compressed in two stages and cooled between them before storing it as liquid hydrogen. Oxygen is also compressed and cooled before storing.

Figure 1 shows us the general overview of the Rankine cycle. The Rankine cycle is an idealized thermodynamic cycle describing the process by which certain heat engines, such as steam turbines or reciprocating steam engines,

allow mechanical work to be extracted from a fluid as it moves between a heat source and heat sink. It forms the foundation of the theories and equations we used for this simulation.

Figure 2 [MD20] shows a schematic of the system that we have used for the simulation.

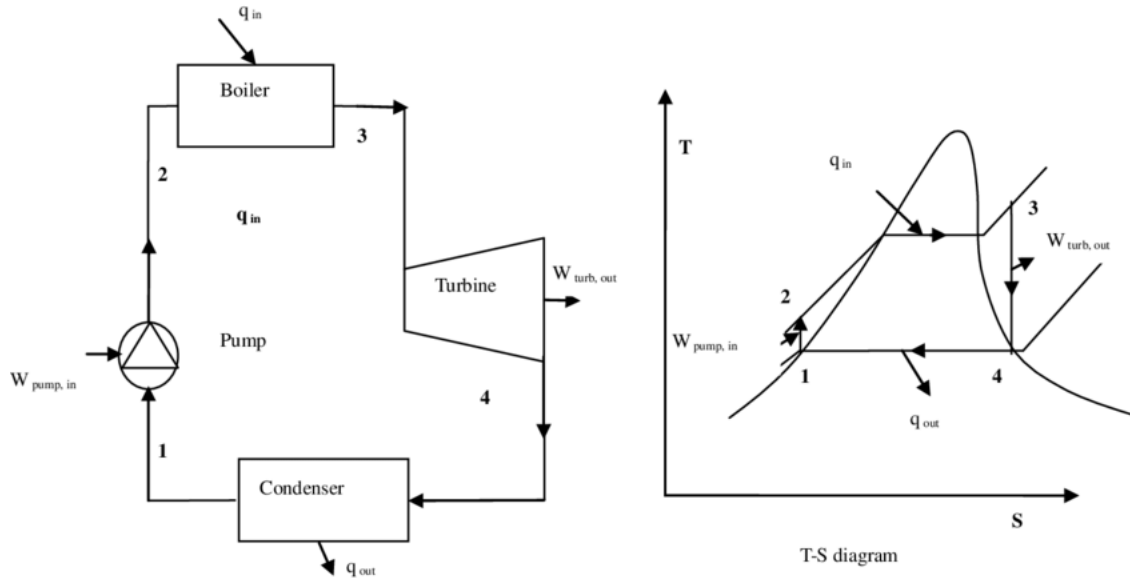


Figure 1: Schematic of Rankine Cycle

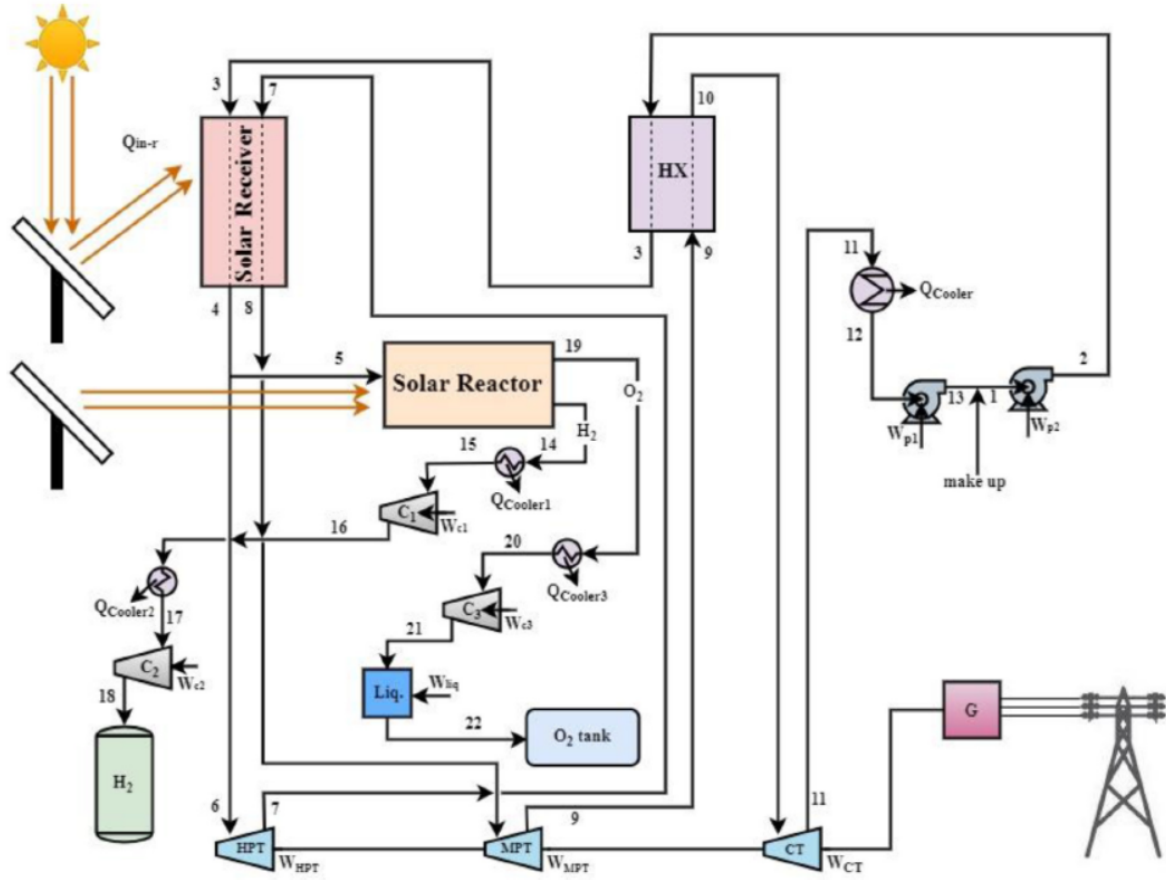


Figure 2: Schematic of the proposed system
[MD20]

7 Equations

Mass, energy, entropy, and exergy balance equations for each component of the proposed system.

Component	MBE	EBE	EnBE	ExBE
Solar Receiver	$\dot{m}_3 = \dot{m}_4$ $\dot{m}_7 = \dot{m}_8$	$\dot{m}_3 h_3 + \dot{m}_7 h_7 + \dot{Q}_{rv} =$ $\dot{m}_4 h_4 + \dot{m}_8 h_8$	$\dot{m}_3 s_3 + \dot{m}_7 s_7 + \frac{\dot{Q}_{in,rv}}{T_{av,rv}} + \dot{s}_{gen,rv} =$ $\dot{m}_4 s_4 + \dot{m}_8 s_8$	$\dot{m}_3 ex_3 + \dot{m}_7 ex_7 + \dot{Q}_{in,rv} \left(1 - \frac{T_0}{T_{av,rv}}\right) = \dot{m}_4 ex_4 +$ $\dot{m}_8 ex_8 + \dot{E}_{x,dest,rv}$
Solar Reactor	$\dot{m}_5 = \dot{m}_{14} + \dot{m}_{19}$	$\dot{m}_5 h_5 + \dot{Q}_{rc} = \dot{m}_{14} h_{14} +$ $\dot{m}_{19} h_{19}$	$\dot{m}_5 s_5 + \frac{\dot{Q}_{rc}}{T_{av,rc}} + \dot{s}_{gen,rc} = \dot{m}_{14} s_{14} +$ $\dot{m}_{19} s_{19}$	$\dot{m}_5 ex_5 + \dot{Q}_{rc} \left(1 - \frac{T_0}{T_{av,rc}}\right) = \dot{m}_{14} ex_{14} + \dot{m}_{19} ex_{19} +$ $\dot{E}_{x,dest,rc}$
HX	$\dot{m}_3 = \dot{m}_2$ $\dot{m}_{10} = \dot{m}_9$	$\dot{m}_2 h_2 + \dot{m}_9 h_9 = \dot{m}_3 h_3 +$ $\dot{m}_{10} h_{10}$	$\dot{m}_2 s_2 + \dot{m}_9 s_9 + \dot{s}_{gen,HX} = \dot{m}_3 s_3 +$ $\dot{m}_{10} s_{10}$	$\dot{m}_2 ex_2 + \dot{m}_9 ex_9 = \dot{m}_3 ex_3 + \dot{m}_{10} ex_{10} + \dot{E}_{x,dest,HX}$
HPT	$\dot{m}_7 = \dot{m}_6$	$\dot{m}_6 h_6 = \dot{m}_7 h_7 + \dot{W}_{HPT}$	$\dot{m}_6 s_6 + \dot{s}_{gen,HPT} = \dot{m}_7 s_7$	$\dot{m}_6 ex_6 = \dot{m}_7 ex_7 + \dot{W}_{HPT} + \dot{E}_{x,dest,HPT}$
MPT	$\dot{m}_9 = \dot{m}_8$	$\dot{m}_8 h_8 = \dot{m}_9 h_9 + \dot{W}_{MPT}$	$\dot{m}_8 s_8 + \dot{s}_{gen,MPT} = \dot{m}_9 s_9$	$\dot{m}_8 ex_8 = \dot{m}_9 ex_9 + \dot{W}_{MPT} + \dot{E}_{x,dest,MPT}$
CT	$\dot{m}_{11} = \dot{m}_{10}$	$\dot{m}_{10} h_{10} = \dot{m}_{11} h_{11} + \dot{W}_{CT}$	$\dot{m}_{10} s_{10} + \dot{s}_{gen,CT} = \dot{m}_{11} s_{11}$	$\dot{m}_{10} ex_{10} = \dot{m}_{11} ex_{11} + \dot{W}_{CT} + \dot{E}_{x,dest,CT}$
Intercooler	$\dot{m}_{12} = \dot{m}_{11}$	$\dot{m}_{11} h_{11} = \dot{m}_{12} h_{12} + \dot{Q}_{cool}$	$\dot{m}_{11} s_{11} + \dot{s}_{gen,cool} = \dot{m}_{12} s_{12} + \frac{\dot{Q}_{cool}}{T_{12}}$	$\dot{m}_{11} ex_{11} = \dot{m}_{12} ex_{12} + \dot{Q}_{cool} \left(1 - \frac{T_0}{T_{12}}\right) + \dot{E}_{x,dest,cool}$
Intercooler 1	$\dot{m}_{15} = \dot{m}_{14}$	$\dot{m}_{14} h_{14} = \dot{m}_{15} h_{15} + \dot{Q}_{cool1}$	$\dot{m}_{14} s_{14} + \dot{s}_{gen,cool1} = \dot{m}_{15} s_{15} + \frac{\dot{Q}_{cool1}}{T_{15}}$	$\dot{m}_{14} ex_{14} = \dot{m}_{15} ex_{15} + \dot{Q}_{cool1} \left(1 - \frac{T_0}{T_{15}}\right) + \dot{E}_{x,dest,cool1}$
Compressor 1	$\dot{m}_{16} = \dot{m}_{15}$	$\dot{m}_{15} h_{15} + \dot{W}_{C1} = \dot{m}_{16} h_{16}$	$\dot{m}_{15} s_{15} + \dot{s}_{gen,C1} = \dot{m}_{16} s_{16}$	$\dot{m}_{15} ex_{15} + \dot{W}_{C1} = \dot{m}_{16} ex_{16} + \dot{E}_{x,dest,C1}$
Intercooler 2	$\dot{m}_{17} = \dot{m}_{16}$	$\dot{m}_{16} h_{16} = \dot{m}_{17} h_{17} + \dot{Q}_{cool2}$	$\dot{m}_{16} s_{16} + \dot{s}_{gen,cool2} = \dot{m}_{17} s_{17} + \frac{\dot{Q}_{cool2}}{T_{17}}$	$\dot{m}_{16} ex_{16} = \dot{m}_{17} ex_{17} + \dot{Q}_{cool2} \left(1 - \frac{T_0}{T_{17}}\right) + \dot{E}_{x,dest,cool2}$
Compressor 2	$\dot{m}_{18} = \dot{m}_{17}$	$\dot{m}_{17} h_{17} + \dot{W}_{C2} = \dot{m}_{18} h_{18}$	$\dot{m}_{17} s_{17} + \dot{s}_{gen,C2} = \dot{m}_{18} s_{18}$	$\dot{m}_{17} ex_{17} + \dot{W}_{C2} = \dot{m}_{18} ex_{18} + \dot{E}_{x,dest,C2}$
Intercooler 3	$\dot{m}_{20} = \dot{m}_{19}$	$\dot{m}_{19} h_{19} = \dot{m}_{20} h_{20} + \dot{Q}_{cool3}$	$\dot{m}_{19} s_{19} + \dot{s}_{gen,cool3} = \dot{m}_{20} s_{20} + \frac{\dot{Q}_{cool3}}{T_{20}}$	$\dot{m}_{19} ex_{19} = \dot{m}_{20} ex_{20} + \dot{Q}_{cool3} \left(1 - \frac{T_0}{T_{20}}\right) + \dot{E}_{x,dest,cool3}$
Compressor 3	$\dot{m}_{21} = \dot{m}_{20}$	$\dot{m}_{20} h_{20} + \dot{W}_{C3} = \dot{m}_{21} h_{21}$	$\dot{m}_{20} s_{20} + \dot{s}_{gen,C3} = \dot{m}_{21} s_{21}$	$\dot{m}_{20} ex_{20} + \dot{W}_{C3} = \dot{m}_{21} ex_{21} + \dot{E}_{x,dest,C3}$
Liquefaction	$\dot{m}_{22} = \dot{m}_{21}$	$\dot{m}_{21} h_{21} + \dot{W}_{liq} = \dot{m}_{22} h_{22}$	$\dot{m}_{21} s_{21} + \dot{s}_{gen,C3} = \dot{m}_{22} s_{22}$	$\dot{m}_{21} ex_{21} + \dot{W}_{liq} = \dot{m}_{22} ex_{22} + \dot{E}_{x,dest,liq}$
Pump 1	$\dot{m}_{13} = \dot{m}_{12}$	$\dot{m}_{12} h_{12} + \dot{W}_{P1} = \dot{m}_{13} h_{13}$	$\dot{m}_{12} s_{12} + \dot{s}_{gen,P1} = \dot{m}_{13} s_{13}$	$\dot{m}_{12} ex_{12} + \dot{W}_{P1} = \dot{m}_{13} ex_{13} + \dot{E}_{x,dest,P1}$
Pump 2	$\dot{m}_1 = \dot{m}_2$	$\dot{m}_1 h_1 + \dot{W}_{P2} = \dot{m}_2 h_2$	$\dot{m}_1 s_1 + \dot{s}_{gen,P2} = \dot{m}_2 s_2$	$\dot{m}_1 ex_1 + \dot{W}_{P2} = \dot{m}_2 ex_2 + \dot{E}_{x,dest,P2}$

Figure 3: Equations used for analysis
[MD20]

The equations that are shown in the table above in Figure 3 are the equations that we used for the simulation that we ran. These equations were translated into the EES format before use.

Figure 4 given below shows us the T-s diagram of the water for developed system. It shows us the relationship between the temperature and the specific enthalpy of the water.

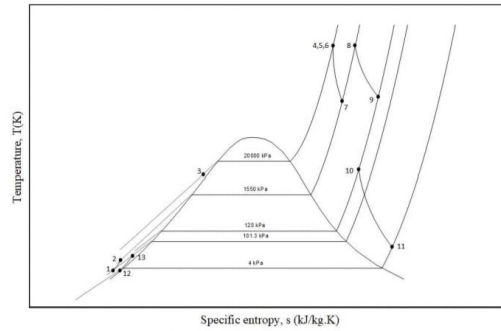


Figure 4: T-s diagram of water of developed system
[MD20]

The values that we used for the equations that we used are given in the table below. These values are the state values. These are the values of each quantity at a specific point in the system. Those values were placed into the equations using EES. The values that we are using for our simulation were all taken from the reference paper.

mass flow rate, \dot{m} (kg/s)	Temperature, T (K)	Specific Enthalpy, h (kJ/kg)	Specific Entropy, s (kJ/kg.K)	Specific Exergy, ex (kJ/kg)
$\dot{m}_1 = 206.6$	$T_1 = 301$	$h_1 = 116.8$	$s_1 = 0.4067$	$ex_1 = 0.06275$
$\dot{m}_2 = 206.6$	$T_2 = 302.8$	$h_2 = 142.3$	$s_2 = 0.4255$	$ex_3 = 20.03$
$\dot{m}_3 = 206.6$	$T_3 = 581.9$	$h_3 = 1381$	$s_3 = 3.289$	$ex_3 = 405.1$
$\dot{m}_4 = 206.6$	$T_4 = 2000$	$h_4 = 6574$	$s_4 = 8.725$	$ex_4 = 3979$
$\dot{m}_5 = 43.5$	$T_5 = 2000$	$h_5 = 6574$	$s_5 = 8.725$	$ex_5 = 3979$
$\dot{m}_6 = 163.1$	$T_6 = 2000$	$h_6 = 6574$	$s_6 = 8.725$	$ex_6 = 3979$
$\dot{m}_7 = 163.1$	$T_7 = 1426.7$	$h_7 = 5027$	$s_7 = 8.999$	$ex_7 = 2350$
$\dot{m}_8 = 163.1$	$T_8 = 2000$	$h_8 = 6587$	$s_8 = 9.915$	$ex_8 = 3637$
$\dot{m}_9 = 163.1$	$T_9 = 1435.5$	$h_9 = 5053$	$s_9 = 10.2$	$ex_9 = 2018$
$\dot{m}_{10} = 163.1$	$T_{10} = 523.15$	$h_{10} = 2973$	$s_{10} = 7.94$	$ex_{10} = 609.4$
$\dot{m}_{11} = 163.1$	$T_{11} = 400$	$h_{11} = 2793$	$s_{11} = 9.003$	$ex_{11} = 60.15$
$\dot{m}_{12} = 163.1$	$T_{12} = 301$	$h_{12} = 116.7$	$s_{12} = 0.4068$	$ex_{12} = 60.15$
$\dot{m}_{13} = 163.1$	$T_{13} = 310$	$h_{13} = 154.4$	$s_{13} = 0.53$	$ex_{13} = 0.9843$
$\dot{m}_{14} = 4.8$	$T_{14} = 2000$	$h_{14} = 30212$	$s_{14} = 95.36$	$ex_{14} = 13770$
$\dot{m}_{15} = 4.8$	$T_{15} = 300$	$h_{15} = 3958$	$s_{15} = 66.79$	$ex_{15} = -3973$
$\dot{m}_{16} = 4.8$	$T_{16} = 800$	$h_{16} = 11226$	$s_{16} = 67.7$	$ex_{16} = 3026$
$\dot{m}_{17} = 4.8$	$T_{17} = 300$	$h_{17} = 3958$	$s_{17} = 53.46$	$ex_{17} = 0.09561$
$\dot{m}_{18} = 4.8$	$T_{18} = 1400$	$h_{18} = 20566$	$s_{18} = 53.48$	$ex_{18} = 16604$
$\dot{m}_{19} = 38.7$	$T_{19} = 2000$	$h_{19} = 1827$	$s_{19} = 2.816$	$ex_{19} = 987.9$
$\dot{m}_{20} = 38.7$	$T_{20} = 300$	$h_{20} = 1.614$	$s_{20} = 0.8453$	$ex_{20} = -250.2$
$\dot{m}_{21} = 38.7$	$T_{21} = 800$	$h_{21} = 493.8$	$s_{21} = 0.939$	$ex_{21} = 214.1$
$\dot{m}_{22} = 38.7$	$T_{22} = 91$	$h_{22} = -187.1$	$s_{22} = 1.076$	$ex_{22} = 133.7$

8 Results and Discussion

Component	w(kW)	Q(kW)	S-gen(kW/K)	Ex.dest(kW)
Compressor 1	34886	-	4.368	1291
Compressor 2	-79718	-	-0.096	-19.66
Compressor 3	19047	-	3.626	1078
Condensing Turbine	38165	-	172.2	51417
High Pressure Turbine	252316	-	44.69	13374
Medium Pressure Turbine	250195	-	46.48	13864
Intercooler	-	427697	18.88	-4263
Intercooler 1	-	126019	282.9	84326
Intercooler 2	-	34886	47.94	14292
Intercooler 3	-	70641	159.2	47444
Pump 1	6149	-	20.09	15799
Pump 2	5268	-	3.884	1143
Heat exchanger	-	-	224.1	150187
Solar receiver	-	1327000	388.6	115639
Solar reactor	-	-70246	221	8601
Liquefaction	-26351	-	5.302	-23239

The table above shows us the values that we have attained from our simulation of the system that we are working with. These values were obtained by using the aforementioned equations and Using EES to solve them. After the simulation was complete we noticed the presence of discrepancies between the values that we have obtained and the expected values as stated in the reference paper. We will be looking into these discrepancies in more detail later.

While attempting to reproduce the paper, we faced some issues In the mathematical analysis part of the paper, and we were wondering if you could give some insights on this. Some discrepancies in the results were observed and it was not negligible, and we thought of letting you know about the

anomalies we encountered. We would be grateful if you could kindly let us know if we have made any mistake in our calculations.

Some of the main issues are:

1. In calculating overall energy efficiency, we couldn't figure out which enthalpy of Oxygen should be used as there were four enthalpies mentioned in the paper.

2. The Higher Heating Value (HHV) of Hydrogen wasn't mentioned in the paper for which we used "142 MJ/kg". We were not sure as to whether or not we should use a different value so that was the one used.

3. Overall energy efficiency of the system is directly proportional to the mass flow rate of Hydrogen, although we utilized the stated equation in the paper, the graphical relation that we obtained showed otherwise.

4. Some of the calculated values of heat, work, entropy generation, and exergy destruction were observed to be negative and/or erroneous when we solved the equations in EES.

5. We were confused about whether we should use the physical, chemical, or total exergies of each state in calculating the specific exergy.

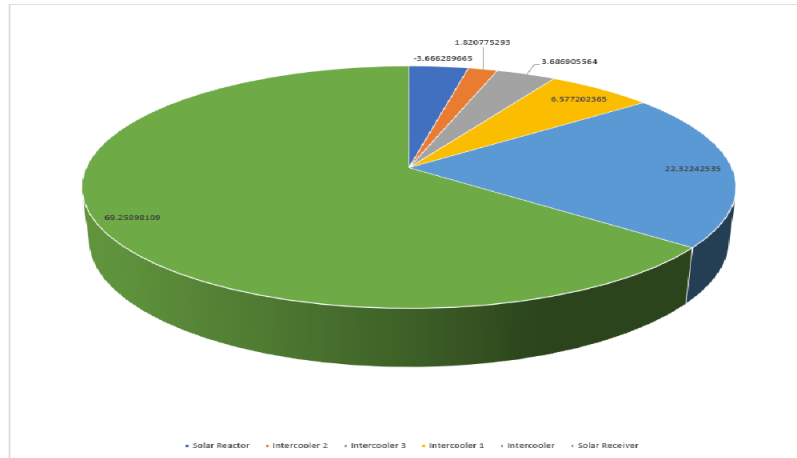


Figure 5: Pie-chart of Power distribution

Given in figures 5 and 6 we can see the power distribution of all the components involved in the system. Figure 4 shows us the distribution in the form of a pie chart. From the chart it is clear to see that the power that is produced by the Solar Receiver is far and wide the greatest amount making up more than half of the chart.

Figure 6 shows us the bar chart of the power consumption/production of the elements in the simulation. From it we can see that the power consump-

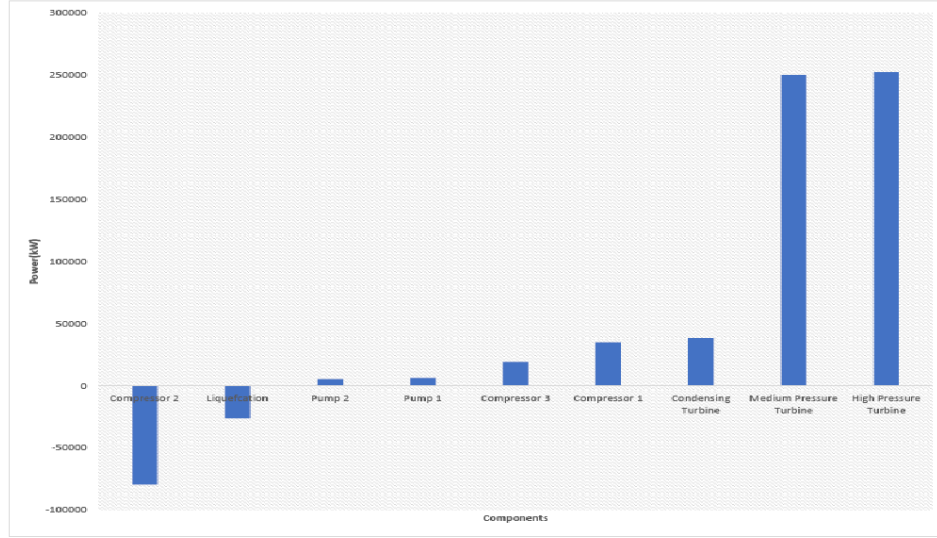


Figure 6: Bar-chart of Power distribution

tion by the compressor and the liquefaction process is substantial. From the bar chart it is also clear to see that the production of power mostly comes from the Medium Pressure and the High Pressure Turbines.

Figure 7 below shows us the rate of change of the Efficiency against the heat rate of the Solar Reactor. The graph shows us the changes of both the Energy and Exergy efficiencies. It is clear to see from the graph that as the Heat rate of the Reactor increases both the Energy and Exergy efficiencies go down. The value of the energy efficiency goes down from about 0.81 to about 0.76 while the value of the exergy efficiency seems to have gone down from just above 0.75 to just above 0.71. Interestingly the rate of change of the efficiencies i.e. the gradients of the lines appear to be rather similar. The relationship between the two variables appears to be one of linear proportionality.

Similar to figure 7, figure 8 shows us the relationship between the Energy and Exergy efficiencies and the Heat rate. However, this time it is the heat rate of the Solar Receiver. Like the previous graph it shows us that the Energy and Exergy efficiencies tend to decrease with the increase of the heat rate, however unlike the previous graph the relationship between the variables is not directly proportional. However one similarity between this graph and the one previous is that the net decrease in the energy and exergy efficiencies are similar.

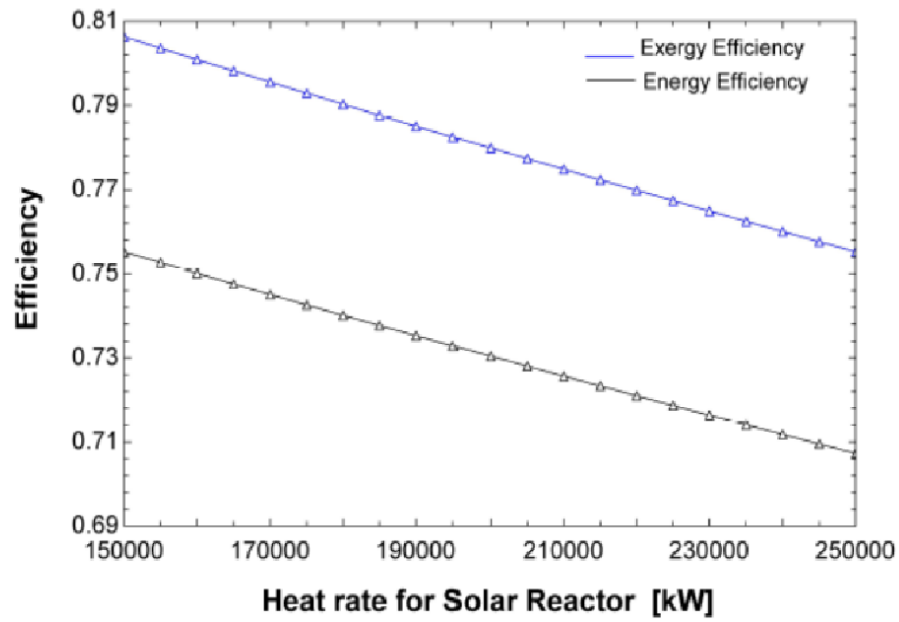


Figure 7: Efficiency vs Heat rate (Reactor)

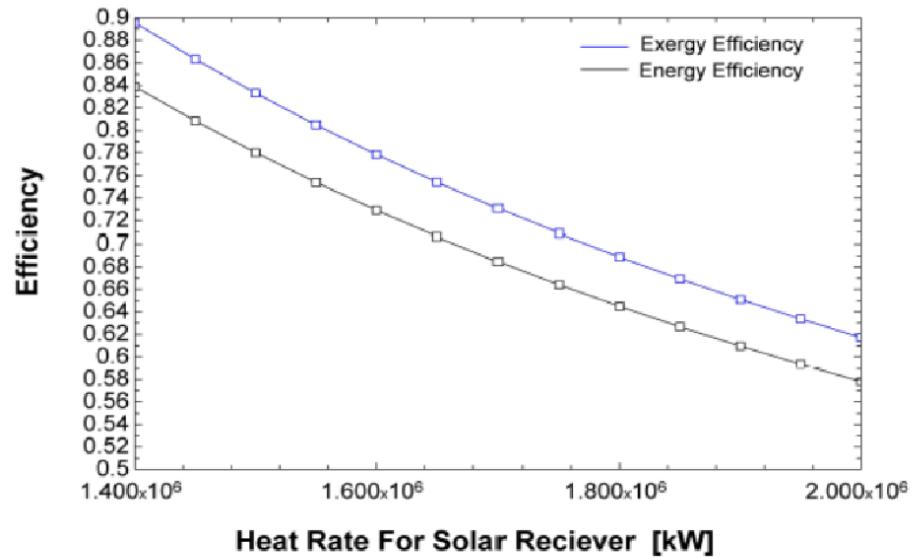


Figure 8: Efficiency vs Heat rate (Receiver)

The graphs below that are illustrated in figures 9 and 10 are especially of interest to us. These are the results that showed the largest discrepancy between the values that we obtained and the values that were present in the reference paper. These graphs display the relationship between the energy and the exergy and the mass flow rate. As we can see in Figure 8 the expected result was to see the efficiencies of both quantities decrease with the mass flow rate however our results were precisely the opposite. According to the simulation we ran the efficiency of both energy and exergy increased with the mass flow rate. Our results are illustrated in Figure 9. Not only that but on figure 8 the net decrease in the energy and exergy efficiencies appear to be quite small. That was not the case in our simulation as our results showed a substantial increase in both the energy and the exergy efficiency.

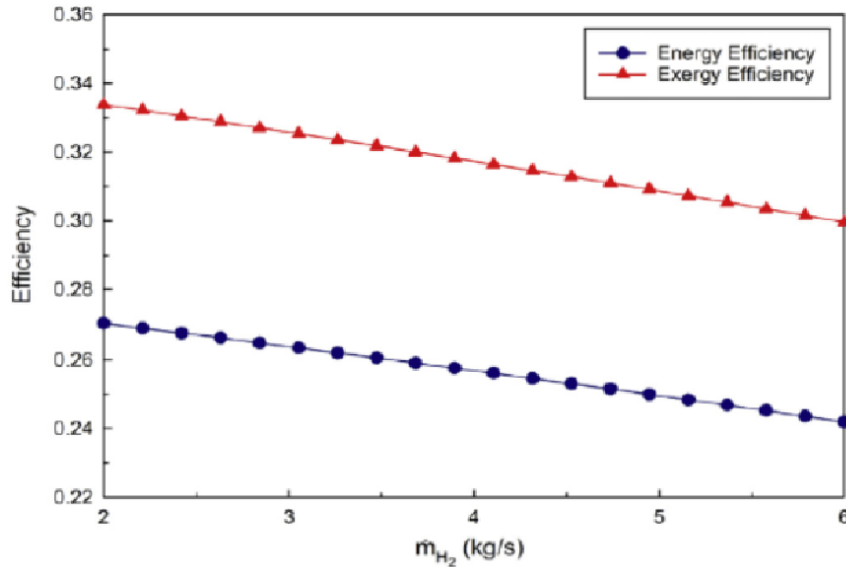


Figure 9: Efficiency vs Mass flow rate (Reference)
[MD20]

In our simulation we found discrepancies between the results that were expected and the results that were obtained. In order to address these discrepancies we reviewed the process of our simulations as well as went over the equations that were used in the simulation. We even contacted the author of the original paper and provided a document of all the issues in order to eliminate the difference. From our findings we concluded that the reference paper that was used is faulty in some manner. However not wanting to proceed under that assumption we made sure to display the results of both instances

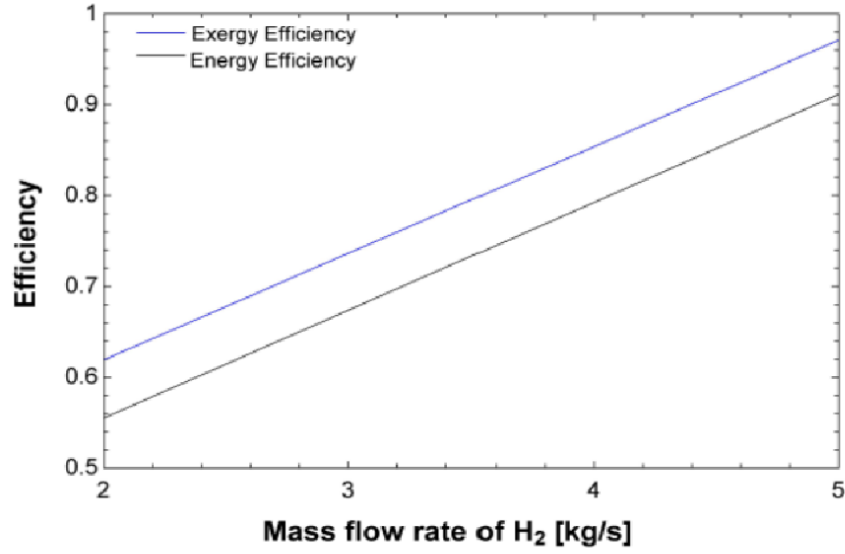


Figure 10: Efficiency vs Mass flow rate (Simulation)

of the simulation and presented a comparison of the results.

Given below are the raw values of the efficiencies that we have obtained from our simulation of the system. As can be seen there is quite a large disparity between the values that we have obtained and the values that we expected to obtain. Our values and the values found on the reference paper are both given and the percentage of error of both the values were calculated and shown to give a better idea of the disparity between results.

Within this table it may be noticed that we have received two percentage error values. That is because we used two different methods of calculation to attain the values. The equations that we used are:

1. $(\text{Value from ref. paper} - \text{Value from simulation}) / \text{Value from ref. paper}$
2. $(\text{Value from ref. paper} - \text{Value from simulation}) / \text{Value from simulation}$

Efficiency	Our Work	From Paper	Calculated using Paper Values	Percentage of error, $\left \frac{\text{Paper} - \text{Sim}}{\text{Paper}} \right $	Percentage of error, $\left \frac{\text{Paper} - \text{Calc}}{\text{Calc}} \right $
Overall Energy Efficiency	89%	25%	64%	254%	38.18%
Overall Exergy Efficiency	96%	31%	71%	210%	34.83%

9 Conclusion

As we have laid out at the beginning of this paper, the world's over reliance on fossil fuels is much cause for concern given the ever-dwindling nature of the resource. Due to this it was imperative that alternative methods of generating energy be researched and implemented as quickly as possible to ensure a sustained quality of life for humankind. For this endeavor we have decided that working on simulating an efficient simulation and system of a renewable energy resource source. Of course we have decided on recreating a previous simulation that was performed in order to verify its accuracy.

With this experiment we have done our level best to ensure that the results we attain are close to the results that were attained in the paper that we used as a reference. However it is clear that that is something that has not occurred. We have noticed some discrepancies between the results that were obtained in the simulation we ran and the results that were obtained by the authors of the simulation paper. We have tried our level best to address the issues that may have resulted in the discrepancies. The causes for those discrepancies are given and discussed in this paper. The overall purpose of the paper was to showcase the system of high temperature, solar driven steam electrolyzer. Through carrying out a thermodynamic analysis we hopefully did an adequate job in showcasing the effectiveness and feasibility of using such a system as an alternative means of energy generation.

10 Appendix

These are the equations that we input into the EES in order to attain the results that we wanted. The format in which the equations are written are identical to the format that is used in the software,

"Work output of the high pressure turbine"

$$W_{hpt} = m_{dot}[6] * h[6] - m_{dot}[7] * h[7]$$

$$m_{dot}[6] * s[6] + s_{genHPT} = m_{dot}[7] * s[7]$$

$$m_{dot}[6] * ex[6] = m_{dot}[7] * ex[7] + W_{hpt} + Ex_{dest_hpt}$$

"Work output of the medium pressure turbine"

$$W_{mpt} = m_{dot}[8] * h[8] - m_{dot}[9] * h[9]$$

$$m_{dot}[8] * s[8] + s_{genMPT} = m_{dot}[9] * s[9]$$

$$m_{dot}[8] * ex[8] = m_{dot}[9] * ex[9] + W_{mpt} + Ex_{dest_mpt}$$

"Work output of the condensing turbine"

$$W_{ct} = m_{dot}[10] * h[10] - m_{dot}[11] * h[11]$$

$$m_{dot}[10] * s[10] + s_{genCT} = m_{dot}[11] * s[11]$$

$$m_{dot}[10] * ex[10] = m_{dot}[11] * ex[11] + W_{ct} + Ex_{dest_ct}$$

"Solar Receiver"

$$m_{dot}[3] * h[3] + m_{dot}[7] * h[7] + Q_{rv} = m_{dot}[4] * h[4] + m_{dot}[8] * h[8]$$

$$m_{dot}[3] * s[3] + m_{dot}[7] * s[7] + Q_{rv}/1501.7 + s_{genRV} = m_{dot}[4] * s[4] + m_{dot}[7] * s[8]$$

$$m_{dot}[3] * ex[3] + m_{dot}[7] * ex[7] + Q_{rv} * (1 - T[0]/1501.7) = m_{dot}[3] * ex[4] + m_{dot}[7] * ex[8] + Ex_{dest_RV}$$

"Solar Reactor"

$$m_{dot}[5] * h[5] + Q_{rc} = m_{dot}[14] * h[14] + m_{dot}[19] * h[19]$$

$$m_{dot}[5] * s[5] + Q_{rc}/2075 + s_{genRC} = m_{dot}[14] * s[14] + m_{dot}[19] * s[19]$$

$$m_{dot}[5] * ex[5] + Q_{rc} * (1 - T[0]/2075) = m_{dot}[14] * ex[14] + m_{dot}[19] * ex[19] + Ex_{dest_RC}$$

"Heat Exchanger"

$$m_{dot}[2] * h[2] + m_{dot}[9] * h[9] = m_{dot}[3] * h[3] + m_{dot}[10] * h[10]$$

$$m_{dot}[2] * s[2] + m_{dot}[9] * s[9] + s_{genhx} = m_{dot}[3] * s[3] + m_{dot}[10] * s[10]$$

$$m_{dot}[2] * ex[2] + m_{dot}[9] * ex[9] = m_{dot}[3] * ex[3] + m_{dot}[10] * ex[10] + Ex_{dest_HX}$$

"Intercooler"

$m_dot[11] * h[11] = m_dot[12] * h[12] + Q_cool$
 $m_dot[11] * s[11] + s_cool = m_dot[12] * s[12] + Q_cool / T[12]$
 $m_dot[11] * ex[11] = m_dot[12] * ex[12] + Ex_dest_cool + Q_cool * (1 - T[0]/T[12])$
 "Intercooler 1"
 $m_dot[14] * h[14] = m_dot[15] * h[15] + Q_cool1$
 $m_dot[14] * s[14] + s_cool1 = m_dot[15] * s[15] + Q_cool1 / T[15]$
 $m_dot[14] * ex[14] = m_dot[15] * ex[15] + Ex_dest_cool1 + Q_cool1 * (1 - T[0]/T[15])$
 "Compressor 1"
 $m_dot[15] * h[15] + W_c1 = m_dot[16] * h[16]$
 $m_dot[15] * s[15] + s_genc1 = m_dot[16] * s[16]$
 $m_dot[15] * ex[15] + W_c1 = m_dot[16] * ex[16] + Ex_dest_c1$
 "Intercooler 2"
 $m_dot[16] * h[16] = m_dot[17] * h[17] + Q_cool2$
 $m_dot[16] * s[16] + s_cool2 = m_dot[17] * s[17] + Q_cool2 / T[17]$
 $m_dot[16] * ex[16] = m_dot[17] * ex[17] + Ex_dest_cool2 + Q_cool2 * (1 - T[0]/T[17])$
 "Compressor 2"
 $m_dot[18] * h[18] + W_c2 = m_dot[17] * h[17]$
 $m_dot[18] * s[18] + s_genc2 = m_dot[17] * s[17]$
 $m_dot[18] * ex[18] + W_c2 = m_dot[17] * ex[17] + Ex_dest_c2$
 "Intercooler 3"
 $m_dot[19] * h[19] = m_dot[20] * h[20] + Q_cool3$
 $m_dot[19] * s[19] + s_cool3 = m_dot[20] * s[20] + Q_cool3 / T[20]$
 $m_dot[19] * ex[19] = m_dot[20] * ex[20] + Ex_dest_cool3 + Q_cool3 * (1 - T[0]/T[20])$
 "Compressor 3"
 $m_dot[20] * h[20] + W_c3 = m_dot[21] * h[21]$
 $m_dot[20] * s[20] + s_genc3 = m_dot[21] * s[21]$
 $m_dot[20] * ex[20] + W_c3 = m_dot[21] * ex[21] + Ex_dest_c3$
 "Liquification"
 $m_dot[21] * h[21] + W_liq = m_dot[22] * h[22]$
 $m_dot[21] * s[21] + s_genliq = m_dot[22] * s[22]$
 $m_dot[21] * ex[21] + W_liq = m_dot[22] * ex[22] + Ex_dest_liq$
 "Water Pump 1"

```

m_dot[12] * h[12] + W_p1 = m_dot[13] * h[13]
m_dot[12] * s[12] + s_genp1 = m_dot[13] * s[13]
m_dot[12] * ex[12] + W_p1 = m_dot[13] * ex[13] + Ex_dest_p1
"Water Pump 2"
m_dot[1] * h[1] + W_p2 = m_dot[2] * h[2]
m_dot[1] * s[1] + s_genp2 = m_dot[2] * s[2]
m_dot[1] * ex[1] + W_p2 = m_dot[2] * ex[2] + Ex_dest_p2
"Overall Energy Efficiency"
eta_enoverall = (eta_hpt * W_hpt + eta_mpt * W_mpt + eta_ct * W_ct -
eta_c1 * W_c1 - eta_c2 * W_c2 - eta_c3 * W_c3 - eta_p1 * W_p1 - eta_p2 *
W_p2 + m_doth2 * HHV + m_dotO2 * h_O2)/(Q_rv + Q_rc)
"Q_rc1 = 210459 [kJ/s]"
"W_comp2 = 80381 [kJ/s]"
eta_hpt = 0.8
eta_mpt = 0.8
eta_ct = 0.8
eta_c1 = 0.8
eta_c2 = 0.8
eta_c3 = 0.8
eta_p1 = 0.95
eta_p2 = 0.95
HHV = 141.8 * 1000 [kJ/kg]
m_doth2 = 4.8 [kg/s]
m_dotO2 = 38.7 [kg/s]
h_O2 = -191 [kJ/kg]
eta_exoverall = (eta_hpt * W_hpt + eta_mpt * W_mpt + eta_ct * W_ct -
eta_c1 * W_c1 - eta_c2 * W_c2 - eta_c3 * W_c3 - eta_p1 * W_p1 - eta_p2 *
W_p2 + m_doth2 * ex_h2 + m_dotO2 * ex_O2)/(Q_rv * (1 - 298/1501.7) +
Q_rc * (1 - 298/2075))
ex_h2 = 118030 [kJ/kg]
ex_O2 = 124.0625 [kJ/kg]

```

In order to remove our doubts regarding the values mentioned in paper, we have used this EES code for calculating the results in the paper

```

"Overall Energy Efficiency according to the values mentioned in the paper"
eta_enoverall = (eta_hpt * W_hpt + eta_mpt * W_mpt + eta_ct * W_ct -
eta_c1 * W_c1 - eta_c2 * W_c2 - eta_c3 * W_c3 -
eta_p1 * W_p1 - eta_p2 * W_p2 + m_doth2 * HHV + m_dotO2 * h_O2)/(Q_rv
+ Q_rc)
"Back Calculation of HHV of H2"
"0.2507= (eta_hpt * W_hpt + eta_mpt * W_mpt + eta_ct * W_ct - eta_c1
* W_c1 - eta_c2 * W_comp2 - eta_c3 * W_c3 -
eta_p1 * W_p1 - eta_p2 * W_p2 + m_doth2 * HHV1 + m_dotO2 * h_O2)/(Q_rv
+ Q_rc)"
"Overall Exergy Efficiency according to the values mentioned in the paper"
eta_exoverall= (eta_hpt * W_hpt + eta_mpt * W_mpt + eta_ct * W_ct -
eta_c1 * W_c1 - eta_c2 * W_c2 - eta_c3 * W_c3 -
eta_p1 * W_p1 - eta_p2 * W_p2 + m_doth2 * ex_h2 + m_dotO2 * ex_O2)/(Q_rv
*(1- 298/1501.7) + Q_rc* (1-298/2075))
"Given Values"
eta_hpt = 0.8
eta_mpt = 0.8
eta_ct = 0.8
eta_c1 = 0.8
eta_c2 = 0.8
eta_c3 = 0.8
eta_p1 = 0.95
eta_p2 = 0.95
HHV = 141.8 * 1000 [kJ/kg]
m_doth2 = 4.8 [kg/s]
m_dotO2 = 38.7 [kg/s]
h_O2 = -191 [kJ/kg]
W_hpt = 252412 [kJ]
W_mpt = 250234 [kJ]
W_ct = 38252 [kJ]
W_c1 = 35180 [kJ]
W_c2 = 80381 [kJ]

```

$$W_{c3} = 19047 \text{ [kJ]}$$

$$W_{p1} = 6155 \text{ [kJ]}$$

$$W_{p2} = 5281 \text{ [kJ]}$$

$$Q_{rc} = 210459$$

$$Q_{rv} = 1327000$$

$$ex_{h2} = 118030 \text{ [kJ/kg]}$$

$$ex_{O2} = 124.0625 \text{ [kJ/kg]}$$

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