Thermodynamic analysis of various electrolysis methods integrated to Small Modular Reactor for hydrogen production

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1. Introduction

The energy production from variable renewable energy (VRE) sources is increasing globally and domestically. Globally, according to the United Nations World Climate Convention, the contribution of renewable energy (RE) is expected to increase to reduce greenhouse gas (GHG) emission. In South Korea, the energy policy 3020 was announced, which aims to increase the contribution of RE (including VRE) to 20% by 2030 [1]. However, as the production from VRE increases, major technical challenges also arise.

Solving the intermittency issue of VRE is one of the major challenges. The power generation from VRE is mostly affected by weather and climate conditions and therefore it cannot always generate power when the demand is high. This issue can be alleviated by load-following operation of a nuclear power plant (NPP). Currently, Small Modular Reactors (SMR) are being developed worldwide because of affordability, safety and sustainability and hydrogen (H₂) production from water electrolysis coupled with SMR can solve this issue.

Hydrogen is considered as one of the most promising clean energy carriers instead of fossil fuels for numerous applications [2]. There are many ways that hydrogen can be produced. Nowadays, hydrogen production via water or steam electrolysis, one of the green hydrogen production methods, is being actively researched. Depending on the temperature of electrolysis, it is classified as low, medium, and high temperature electrolysis methods. The concepts and layouts of electrolysis method coupled with SMR are different depending on its temperature.

Steam electrolysis using an NPP was studied and analyzed previously [3]. The previous study presented the hydrogen production from steam electrolysis using heat and electricity of an NPP. According to this work, the efficiency of hydrogen production increases as the electrolysis temperature increases.

Therefore, in this paper, thermodynamic analysis and concepts of various hydrogen production methods from steam electrolysis using SMR are presented. The performances of hydrogen production under various conditions such as temperature and steam bypass fraction in terms of the hydrogen production efficiency are predicted and compared.

2. Thermodynamic modeling

2.1 Description of steam electrolysis using SMR

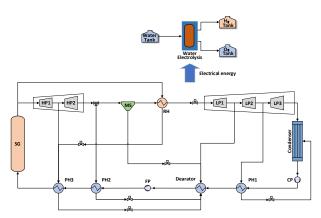


Figure 1. Layout of low temperature water electrolysis (LTE) using SMR

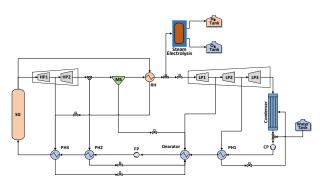


Figure 2. Layout of medium temperature steam electrolysis (MTSE) integrated to steam cycle of SMR

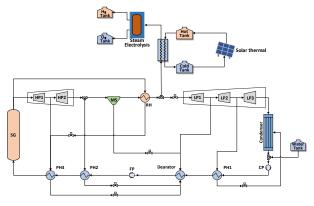


Figure 3. Layout of high temperature steam electrolysis (HTSE) integrated to steam cycle of SMR

J.H. Park [4] investigated the part-load performance analysis of an SMR integrated with thermal energy storage. The concept and thermodynamic modeling of the steam cycle for SMR in the reference is used in this paper. Figures 1, 2 and 3 show the layout of low, medium and high temperature steam electrolysis with SMR. Firstly, the low temperature water electrolysis (LTE) is generating hydrogen from electrolysis occurring at room temperature to less than 100°C. It is noted that the low temperature water electrolysis does not require steam from the steam cycle of an SMR since it is integrated to an SMR only electrically.

Next, the medium temperature steam electrolysis (MTSE) has electrolysis temperature from 100° C to 400° C. The steam bypassed from the steam cycle of an SMR flows to steam electrolysis and is used for hydrogen production. Water is supplied to condenser of an SMR to make up for the steam bypass. The point to bypass steam is set to the inlet of low-pressure turbine (LPT), with the temperature close to 300° C [4].

Finally, high temperature steam electrolysis (HTSE) operates in between 700°C and 1000°C. A heater to increase the temperature of the steam is added since the temperature of bypassed steam is near 300°C.

2.2 Thermodynamic modeling

Assumptions used for the modeling are as follows:

(1) Water, hydrogen and oxygen tanks are at the same temperature, pressure.

(2) There is no pressure drop in the pipelines.

(3) There are no changes in potential and kinetic energies.

The enthalpy of reaction (ΔH) consists two parts as shown in the below equation. ΔG is the Gibbs free energy of reaction and has to be applied in the form of electricity. This is also called the change in Gibbs free energy. Then, Q is the product of the thermodynamic temperature (T) and the entropy of reactions (ΔS) and can be applied in the form of thermal energy.

$$\Delta H(T,p) = \Delta G(T,p) + Q(T,p)$$

As shown in the equation below, it is required to know the Gibbs free energy for the specific temperature. The Gibbs free energy can be obtained by using partial pressure information. Thus, by using Kirchhoff's equation, entropy equation and thermodynamic data, the Gibbs free energy can be calculated [3] as shown in the following equation. Figure 4 shows voltages depending on temperature and

pressure, which are results calculated from the below equation.

$$\Delta G(T,p) = \Delta G(T,p^0) + RT \ln[\frac{(\frac{p_{O_2}}{p^0})^{\frac{1}{2}}(\frac{p_{H_2}}{p^0})}{(\frac{p_{H_2}o}{p^0})}]$$

Since the mass flow rate of LP turbine inlet was changed from the nominal mass flowrate due to steam bypass, an off-design model for the LPT is applied to evaluate the lost work [4]. When branching the flow rate and applying the off-design model, the temperatures and pressures in the steam cycle change, so the SG inlet temperature will be different from the nominal condition. Since it is intended to minimize effect on the primary side of SMR while producing hydrogen, the steam cycle conditions was optimized to maintain SG inlet condition at the nominal condition. As a result of this approach, a control valve is installed to adjust the branch flow at the high-pressure turbine outlet.

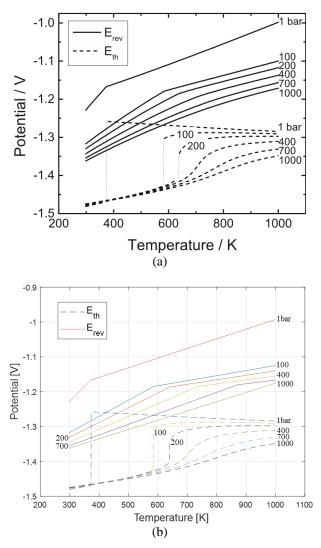


Figure 4. Reversible and thermoneutral voltages according to temperature and pressure of previous study (a) and this study (b)

2.3 Modeling parameters

The design parameters are shown in Table 1 and the variables and ranges of variation are shown in Table 2. In this paper, steam bypass fraction means the ratio of mass flowrate of bypassed steam for hydrogen production and the mass flowrate of LPT inlet.

Table1. Design parameters

Type of Electrolysis	Parameters	Value	Unit
LTE	Temperature of water tank	25	°C
	Pressure of water tank	0.101	MPa

MTSE & HTSE	Temperature of bypassed steam	300	°C
	Pressure of bypassed steam	1.4	MPa
_	Molar mass of water	18	g/mol
All	Molar mass of oxygen	16	g/mol
Electrolysis –	Molar mass of hydrogen	2	g/mol
Liectiolysis –	HHV of hydrogen (Higher Heating Value)	285.8	kJ/mol
Table2. Variables			
Type of Electrolysis	Variables	Range	Unit
LTE	Temperature of water electrolysis	25-99	°C
MTSE	Steam bypass fraction	4-40	%
HTSE	Temperature of steam electrolysis	700-1000	°C
	Steam bypass fraction	4-40	%

3. Thermodynamic evaluation and Results

An efficiency of hydrogen production (η_{H_2}) is the ratio of the energy carried by unit amount of produced hydrogen, which is the higher heating value of hydrogen (HHV=285.8kJ/mol), to the $Q_{overall}$ in the process of hydrogen production. Thus, the efficiency of hydrogen production in this system can be calculated using the next equation [5, 6, 7],

$$\eta_{H_2} = \frac{HHV}{Q_{overall}}$$

$$= \frac{HHV}{Q_{e,Electrolysis} + Q_{th,Electrolysis} + Q_{th,HX} + Q_{work,loss}}$$

where $Q_{e,Electrolysis}$, $Q_{th,Electrolysis}$, $Q_{th,HX}$ and $Q_{work,loss}$ represent the thermal energy to produce electricity energy from electrolysis, heat from electrolysis, heat from heat exchanger to make the high-temperature steam electrolysis and the thermal energy to produce work loss of SMR due to bypassed steam, respectively. $Q_{e,Electrolysis}$ and $Q_{work,loss}$ are further defined with the next equations.

$$Q_{e,Electrolysis} = \frac{E_{e,Electrolysis}}{\eta_{Net,SMR}}$$
$$Q_{work,loss} = \frac{W_{work,loss}}{\eta_{net,SMR}}$$

where $E_{e,Electrolysis}$, $W_{work,loss}$ and $\eta_{net,SMR}$ represent the electricity energy from electrolysis, work loss of SMR due to bypassed steam and net efficiency of SMR depending on steam bypass fraction, respectively.

LTE does not require heat input since it is not be practical or efficient compared to using electrical energy alone [8]. Therefore, using only electrical energy is generally preferred for low temperature water electrolysis. Thus, in LTE, using only electrical energy is considered and the efficiency is quite low. As shown in Figure 5 and Figure 6, the efficiency of H₂ production is 27.5% and the required energy for the production is 144kWh/kg. Efficiency increases only slightly with increasing temperature. The energy required to produce 1 kg of H_2 decreases slightly with increasing temperature. In other words, the temperature does not strongly influence the overall process.

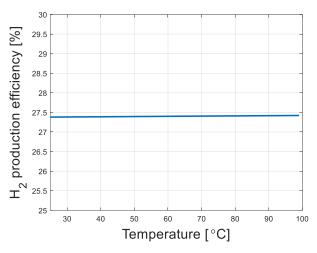


Figure 5. Temperature of electrolysis vs Efficiency of H_2 production in LTE

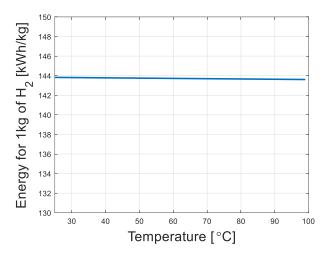


Figure 6. Temperature of electrolysis vs Energy for 1kg of H₂ in LTE

In MTSE and HTSE, unlike LTE, the steam from the steam cycle of an SMR is directly used for the steam electrolysis. Off-design analysis of the steam cycle and maintaining the inlet temperature of steam generator (SG) have to be considered for these two methods. Figure 7 shows that SG inlet temperature is kept constant although the steam is bypassed for the hydrogen production. The off-design model is applied for the evaluation.

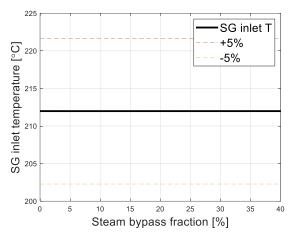


Figure 7. Steam bypass fraction vs SG inlet temperature of SMR

In Figures 8 and 9, as steam bypass fraction increases, both the LPT work and the net efficiency of an SMR decrease. By the definition of hydrogen production efficiency, these affect the efficiency quite much. This is because electricity is the largest energy required for the steam electrolysis. Moreover, the degradation of net efficiency makes the required energy to be larger. From the previous work [4], the net efficiency of SMR for evaluating the efficiency of hydrogen production is estimated with the following equation;

$$\eta_{Net,SMR} = \frac{W_{turb,SMR} - W_{pump,SMR}}{Q_{in,SMR}}$$

where $W_{turb,SMR}$, $W_{pump,SMR}$ and $Q_{in,SMR}$ represent the produced work by turbine, the required work by pump and the heat transferred from primary loop of SMR, respectively.

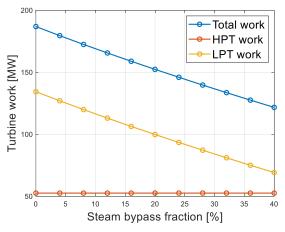


Figure 8. Steam bypass fraction vs HPT, LPT and total work of SMR

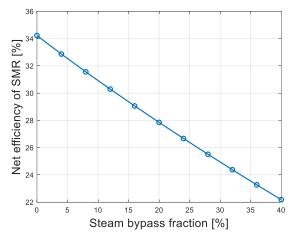


Figure 9. Steam bypass fraction vs Net efficiency of SMR

As shown in Figure 10, MTSE has the efficiency of H_2 production of 20-30%. As the steam bypass fraction increases, the efficiency decreases. Compared to the temperature effect on LTE, the steam bypass fraction has larger effect on H_2 efficiency. It is noted that in this study, the range of steam bypass fraction is set to 4-40%. In Figure 11, as the steam bypass fraction increases, the required energy to produce 1kg of hydrogen increases. In other words, it means that it needs more unit energy for producing 1kg of hydrogen. In MTSE, minimum required energy for hydrogen production is 122kWh/kg.

However, both the required electrical energy and the produced work from SMR should be considered since the required electrical energy should not be more than the produced work from SMR. Figure 12 shows the required energy and the produced work with respect to the steam bypass fraction. In MTSE, the steam bypass fraction cannot be more than 8% since the electrical energy requirement for hydrogen production will exceed when more than 8% of steam is bypassed to MTSE.

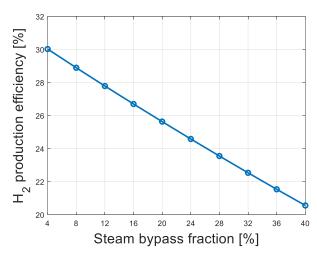


Figure 10. Steam bypass fraction vs Efficiency of $H_{\rm 2}$ production in MTSE

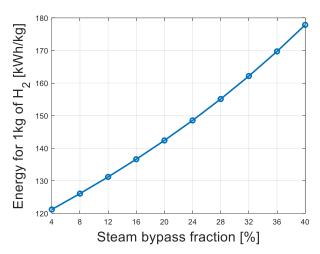


Figure 11. Steam bypass fraction vs Energy for 1kg of H₂ in MTSE

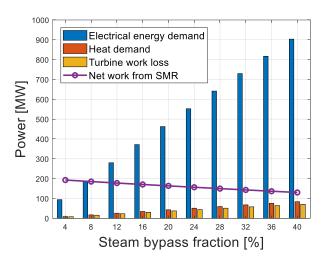


Figure 12. Electrical energy, heat, turbine work loss and net work from SMR depending on Steam bypass fraction in MTSE

As shown in Figure 13, HTSE has the H_2 production efficiency of 22-31%. As the steam bypass fraction increases, the efficiency decreases. It shows small changes in hydrogen efficiency with temperature. In other words, the steam bypass fraction is dominant factor than the temperature on the hydrogen production efficiency. Similar to MTSE, the steam bypass fraction has larger effect on hydrogen efficiency than temperature. Figure 14 shows the trends of required energy to produce 1kg of hydrogen depending on temperature and steam bypass fraction. The trends are similar with LTE and MTSE. The required energy is 118kWh/kg.

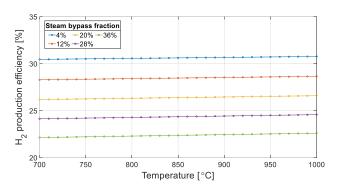


Figure 13. Temperature of steam electrolysis vs Efficiency of H₂ production in HTSE

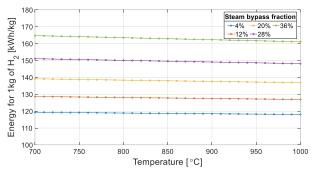
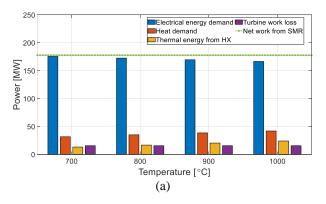


Figure 14. Steam bypass fraction vs Energy for 1kg of H₂ in HTSE

Compared with hydrogen efficiency of LTE and MTSE, that of HTSE is slightly higher. The required electrical energy is compared to the produced work from an SMR for HTSE. Figure 15 shows various types of energy and work depending on electrolysis temperature with 8% and 12% steam bypass fraction. As the temperature decreases, the required electrical energy decreases. This means that it is possible to bypass more steam for higher electrolysis temperature. In Figure 15 (a), it shows that the produced work is larger than the required electrical energy for 8% steam bypass fraction case. However, in Figure 15 (b), the required electrical energy is larger than the produced work for 12% steam bypass fraction. Thus, even with HTSE, it is expected that the steam cannot be bypassed to the hydrogen production more than 8~10% if only nuclear electricity is used for the hydrogen production.



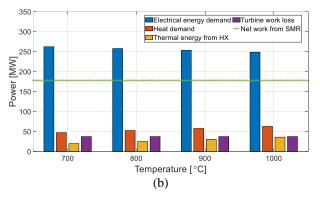


Figure 15. Electrical energy, heat, turbine work loss and net work from SMR depending on temperature with 8% steam bypass fraction (a) and 12% steam bypass fraction (b) in HTSE

4. Summary and Future works

From the results of this study, it is shown that as the electrolysis temperature increases, the efficiency of H_2 production increases but the effect is less dominant than how much steam is diverted to the hydrogen production from the steam cycle. The maximum efficiency of hydrogen production is observed for the high temperature steam electrolysis reaching 31% efficiency at 4% steam bypass fraction and 1000°C operating temperature.

In this study, it is newly observed that when the steam is bypassed from the steam cycle for the hydrogen production, both medium and high temperature steam electrolysis methods cannot accept more than 8% of the total mass flowrate since the steam bypass fraction increases more than that value the electrical power required by the hydrogen production will exceed the electrical power generated from the steam cycle of an SMR. Thus, if more steam is to be bypassed to the hydrogen production from an SMR is necessary, electrical power supplied from other power source such as other nearby SMRs or VRE have to be considered.

Further investigation will be directed towards the economic analysis of steam electrolysis integrated to an SMR. The work will compare the economic values of hydrogen production and the required energy and work losses. Moreover, the hydrogen production will be compared to other energy storage methods as well to determine the best energy storage method for an SMR.

Acknowledgement

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REFERENCES

[1] 산업통상자원부, 제 9 차 전력수급기본계획(2020~2040), 2020

[2] Renato S, Domenico G, Claudia T, Carlo T. Modelling of hydrogen sulfide dispersion from the geothermal power plants of Tuscany (Italy). Sci Total Environ 2017;583:408-20. [3] YongJae Chae et al. "Preliminary analysis of hydrogen production of water electrolysis using NPP" Transactions of the Korea Nuclear Society Autumn Meeting (2022).

[4] Jung Hwan Park, Jeong Ik Lee. "Part-load performance analysis of Small Modular Reactor integrated with thermal energy storage." Proceedings of ICAPP, 2023.

[5] Smolinka T, Ojong ET, Garche J. Hydrogen production from renewable energies—electrolyzer technologies. Electrochem Energy Storage Renew Sources Grid Balanc 2015:103–28.

[6] Mingyi L, Bo Y, Jingming X, Jing C. Thermodynamic analysis of the efficiency of high-temperature steam electrolysis system for hydrogen production. J Power Sources 2008;177:493e9

[7] B. Yildiz, M.S. Kazimi, Int. J. Hydrogen Energy 31 (2006) 77–92.

[8] Rashid, Mamoon & Al Mesfer, Mohammed & Naseem, Hamid & Danish, Mohd. (2015). Hydrogen Production by Water Electrolysis: A Review of Alkaline Water Electrolysis, PEM Water Electrolysis and High Temperature Water Electrolysis. International Journal of Engineering and Advanced Technology. ISSN. 2249-8958.