

Development of Computational Model of High Temperature Steam Electrolysis with Nuclear Energy for Hybrid Energy System

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1. Introduction

Energy Industry has been experiencing huge transformation for reducing the greenhouse gas emission and enhancing energy security. As a clean energy source, the nuclear energy has been regaining the attention and required versatile roles, e.g., flexible power operation, industrial heat application, hydrogen production. Note that the electrolysis with nuclear energy has been recognized as the most viable clean hydrogen production method. [1] Especially, the large-scale high temperature electrolysis (HTE) has been investigated via demonstration projects.

The integration of nuclear energy and hydrogen electrolysis has significant benefits for the energy industry. Basically, the electricity generated by nuclear power plant can be used for electrolysis. Depending on the net electricity demand and electricity price, the electricity output of nuclear power plant could be adjusted by extracting steam for hydrogen production while the reactor operated constantly in the full power. This means the hydrogen production plant could be utilized as a flexible resource for stabilizing energy system and hydrogen could be used as a clean energy carrier.

In particular, the small modular reactor (SMR) has various advantages in utilizing process heat because of its enhanced safety, load-following capability and modular construction. It could be constructed near application plants; thus, it minimizes the loss in transmission of energy (e.g., electricity, heat), enhance the financial investment affordability, and improve the energy utilization efficiency and economic revenue. Therefore, SMR has been considered as an important candidate for coupling with industrial applications in the future nuclear market.

However, the competitiveness of hydrogen production with nuclear energy should be examined technically as well as economically. The environmental factors (e.g., net demands, industrial condition, hydrogen usages) would vary by regions and by countries. The sizing the nuclear power plant and hydrogen production plants and operator strategies should be carefully determined based on the scenario analysis.

In order to estimate the benefits and competitiveness of hydrogen production using nuclear energy,

computational analysis should be necessary. A dynamic behavior should be analyzed for optimizing system/component design and those control/operation strategies. In this study, the Solid Oxide Electrolyzer Cell (SOEC) module is developed and integrated with the previously developed SMART SMR [2,3] model by using Modelica [4]. The mathematical formula is applied to the SOEC model to calculate the amount of hydrogen produced according to vapor injected rate and the temperature conditions. Using this integrated model, the coupled physical behavior of nuclear power plant and hydrogen production plant could be evaluated and optimized configuration could be determined. Ultimately, the optimum operation strategy could be proposed by considering the economic analysis.

2. Development of the Computational Model

2.1 Development of the SOEC Module

The SOEC model has been developed using Modelica. Fig.1 and Fig.2 present the schematic of the SOEC and Modelica SOEC module, respectively. As the steam and electrical energy are supplied, water is decomposed at the porous cathode to generate hydrogen. Meanwhile, oxygen ions pass through the electrolyte and move to the anode to be converted into oxygen molecules [5].

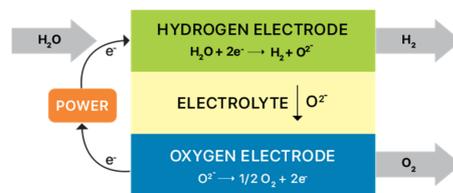


Fig.1 Schematic of SOEC



Fig.2 Modelica SOEC Module

The SOEC cell voltage required for water electrolysis is presented in as follows [6].

$$V = E + \eta_{conc} + \eta_{act,c} + \eta_{act,a} + \eta_{ohmic}$$

E	equilibrium voltage [V]
η_{conc}	concentration overpotential [V]
$\eta_{act,c}$	activation overpotential at cathode [V]
$\eta_{act,a}$	activation overpotential at anode [V]
η_{ohmic}	ohmic overpotential [V]

The overpotential is related with partial pressure of the steam, oxygen, and hydrogen in the SOEC cell. Partial pressure can be calculated as follows [4].

$$m_{SOEC} = \int (\dot{m}_m - \dot{m}_{out}) dt$$

m_{SOEC}	total mass in cell [kg]
\dot{m}_m	total inflow rate in cell [kg/s]
\dot{m}_{out}	total outflow rate in cell [kg/s]

$$\dot{m}_{out} = A_{out} \rho_{avg} \sqrt{\frac{2 \times P_{SOEC}}{\rho_{avg}}}$$

A_{out}	outflow area [m ²]
ρ_{avg}	average density in cell [kg/ m ³]
P_{SOEC}	total pressure in cell [Pa]

$$mole_{SOEC} = m_{SOEC} \times 1000 / M_{cell}$$

$mole_{SOEC}$	total mole in cell [mole]
M_{cell}	average molar weight in cell [g/mole]

$$P_{SOEC} \times V_{cell} \times N_{cell} = mole_{SOEC} \times R \times T_{SOEC}$$

V_{cell}	volume of cell [m ³]
N_{cell}	number of the cell [#]
R	gas constant [J/K-moll]

$$P_{SOEC} = P_{H_2} + P_{O_2} + P_{N_2} + P_{STEAM}$$

P_{H_2}	partial pressure of hydrogen
P_{O_2}	partial pressure of oxygen
P_{N_2}	partial pressure of nitrogen
P_{STEAM}	partial pressure of steam

The efficiency of the SOEC cell is presented in as follow.

$$\eta_{cell} = \frac{E}{E + \eta_{conc} + \eta_{act,c} + \eta_{act,a} + \eta_{ohmic}}$$

η_{cell}	efficiency of the SOEC cell
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According to the power applied to the SOEC cell current can be calculated as follows.

$$I_{cell} = \frac{P_{cell}}{V} \eta_{cell}$$

I_{cell}	current applied to the cell
P_{cell}	power applied to the cell

Hydrogen mass production rate is presented in as follow.

$$\dot{m}_{H_2} = \frac{M_{H_2} I_{cell}}{zF \times 1000}$$

M_{H_2}	molar weight of hydrogen [g/mole]
F	Faraday constant = 96485.33 [C/mol]

2.2 SMART – SOEC Integrated modeling & Simulation

The SOEC module is integrated with the previously developed SMART model by using the Modelica simulation program. Fig.3 presents the schematic of the SMART-SOEC integrated model.

Steam on the secondary side is extracted from the inlet of the high-pressure turbine and steam is produced through heat exchange. In addition, additional heat is applied to steam by an electrical heater to supply steam of 700°C or higher to the SOEC Module. The produced hydrogen from SOEC is stored in a hydrogen storage tank.

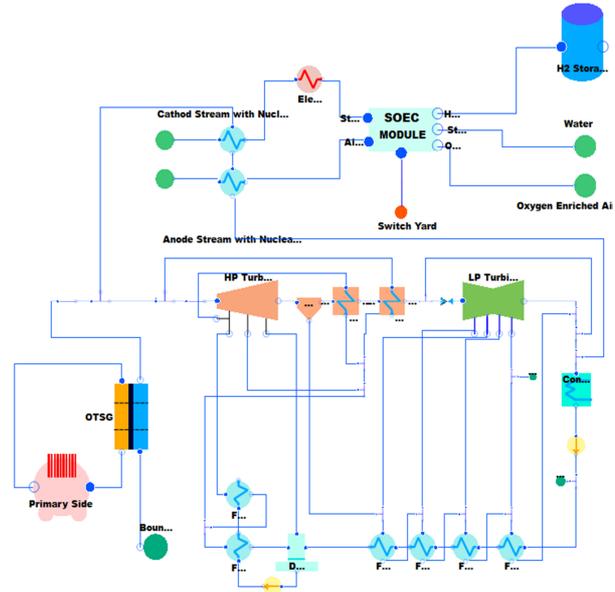


Fig.3 Schematic of the SMART-SOEC Integrated Model

(1) Hydraulic System Sizing

Based on the 5% steam extraction that does not affect the operation of the power plant [7], the calculation of the proper flow rate of water to the SOEC is conducted. The extracted steam is condensed in the shell side of the heat exchanger, and water supplied to the SOEC is

boiled in tube side. The specifications of the intermediate heat exchanger (IHX) are as follows.

- Type: Once through type
- Tube ID / OD: 3mm / 5mm
- Number of Tube: 200 EA

The proper flow rate to the SOEC is determined by calculating enthalpy of the steam (Table I).

Table I. Outlet Enthalpy of Heat Exchanger

The flow rate of the water to the SOEC [kg/s]	Outlet Enthalpy of Heat Exchanger [kJ/kg]
1	2791 (superheated)
2	2728 (superheated)
3	2479 (steam water mix)

The proper flow rate of water to the SOEC has been determined as 2 kg/s because the superheated steam condition is maintained and sufficient flow rate can be supplied.

(2) Determination of the SOEC Cell Capacity

Standard potential in volt (E_0) can be presented as follow.

$$E_0 = 1.253 - 2.4516 \times 10^{-4} \times T_{SOEC}$$

At a typical 700°C temperature in high-temperature water electrolytes, E_0 is calculated as 1.08V. The maximum current at 1000W of power supplied to each cell is calculated as follows.

$$I_{cell} = \frac{P_{cell}}{V} = \frac{1000}{1.08} = 925.9A$$

The required steam supply per cell is calculated as follow.

$$\dot{m}_{H_2O} = \frac{M_{H_2O} I_{cell}}{zF \times 1000} = \frac{18 \times 925.9}{2 \times 96485 \times 1000} = 8.63E - 5 kg$$

Since the flow rate of steam to the SOEC is 2kg, the proper number of the SOEC Cell is determined as follow.

$$\frac{2kg}{8.63E - 5kg / cell} = 23,174$$

The Number of SOEC cell is determined as 25,000, conservatively.

(3) Hydrogen Production in Steady State

Based on the sizing results and the derived SOEC capacity, the amount of hydrogen produced in a steady-state is evaluated. The analysis is conducted under the following conditions..

- Heater Power: 2 MW
- Applied Power to SOEC: 25 MW
- Tube Inlet Temperature: 20 °C
- Tube Inlet Pressure: 1 bar
- Shall Inlet Temperature: 271.76 °C
- Shall Inlet Pressure: 49.46 bar

The SOEC parameter in constant power operation is presented in Table II. The amount of the hydrogen production is calculated as 13,917 kg/day. And required electricity is calculated as follow.

$$\begin{aligned} \text{Required Electricity} &= \\ &= \frac{(\text{Heater Power} + \text{Electric Power applied to SOEC}) / \text{Hydrogen Mass}}{13917kg / day} \\ &= \frac{(25MW + 2MW) \times 1000(kW / MW) \times 24h / day}{13917kg / day} \\ &= 46.56kWh_e / kg \end{aligned}$$

Table II. SOEC Parameter in Constant Power Operation

Parameter		Value
Partial Pressure In SOEC Cell [bar]	Hydrogen	0.252
	Oxygen	0.126
	Steam	1.078
SOEC Cell Temperature [°C]		723.86
SOEC Cell Efficiency		0.674
Hydrogen Mass in Hydrogen Storage Tank for 1 day [kg]		13,917
Hydrogen Tank Pressure on 1 day [bar] (Initial Pressure: 1 bar)		18.12
Electricity Required [kWh _e /kg-H ₂]		46.56

(4) Changes on the primary side for steam extraction

During steam extraction from HP turbine inlet, the flow rate in the SG secondary side increases, and the more heat of the primary side is removed and the reactivity increases by reactivity feedback mechanisms. The effect on the primary side is evaluated under 10% steam extraction condition.

As the flow rate is increased by 10% for 100~200 seconds (Fig.4), the reactivity is increased by 7.0e-6 (Fig.5) due to enhanced heat transfer and lower the core inlet temperature. The core power is increased from 365 MW to 370.3 MW (Fig.6) and the fuel temperature is increased as 0.25°C (Fig.7). The system responses would occur during the short period of time of initiating steam extraction, and the system would be stabilized quickly.

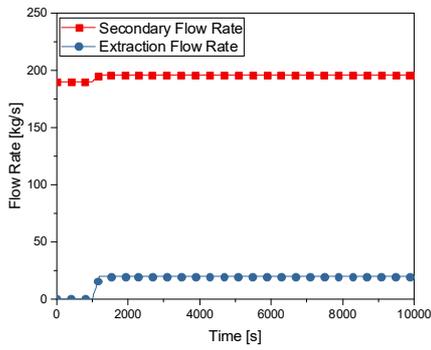


Fig.4 The change of the Steam Extraction and Secondary Flow Rate

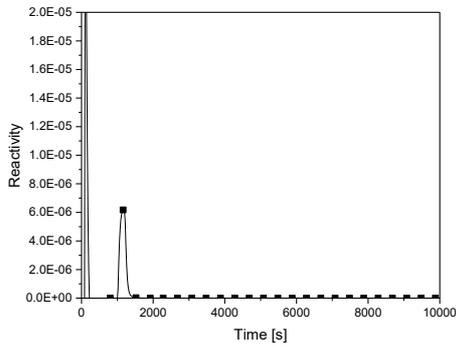


Fig.5 The change of the Reactivity

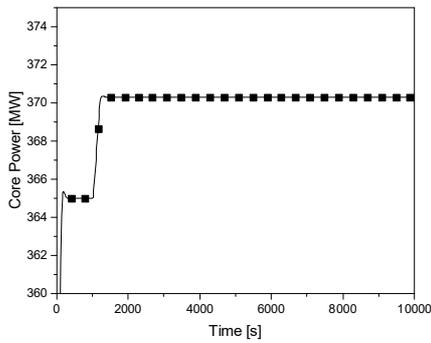


Fig.6 The change of the Core Power

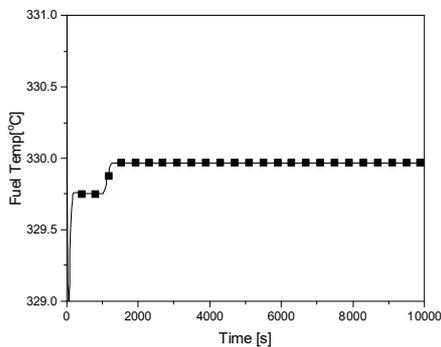


Fig.7 The change of the Fuel Temperature

(5) Hydrogen Production according to changes in the power supplied to SOEC

Hydrogen production is evaluated when the power supplied to SOEC is changed. During the daytime (9 am to 5 pm), the amount of renewable energy generated by photovoltaic power generation is larger. So in daytime, more power is used into SOEC to produce hydrogen. The power used in the SOEC is as follows (Fig.8).

- 9 am ~ 5 pm: 30 MW
- 5 pm ~ 9 am: 5 MW

The SOEC efficiency and the amount of the hydrogen production are presented in Fig.9 & Fig.10, respectively.

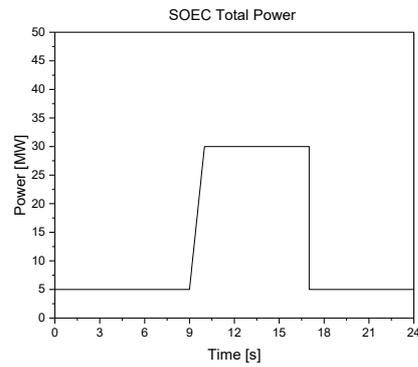


Fig.8 Power used for SOEC for one day

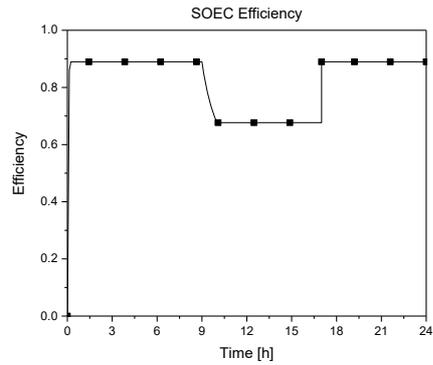


Fig.9 The efficiency change of SOEC Cell

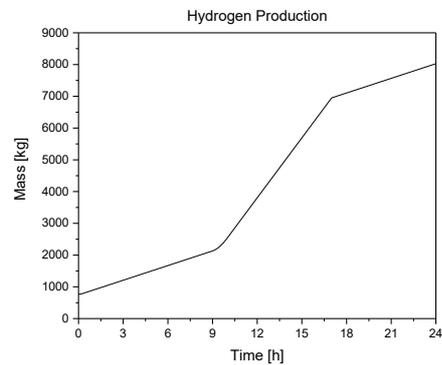


Fig.10 Produced Hydrogen

5. Conclusions

The SMART-SOEC integrated theoretical model has been developed using Modelica. The SOEC module is integrated with the previously developed SMART model. And the analyses are conducted under various conditions. The performance and specifications of the SMART-hydrogen plant derived through analysis are summarized in Table III.

In further study, the developed Modelica model will be benchmarked with actual experiment data of the SOEC module. And it will be used to evaluate the economic feasibility of hydrogen production using nuclear power.

Table III. The Performance and Specification of the SMART-Hydrogen Production Plant

Specification	Value
Extracted Stream Flow Rate	9.52 kg/s (5% Extraction)
The Number of the SOEC Cell	25,000
IHX Exchanger	
Tube ID	3 mm
Tube OD	5 mm
Number of Tube	200 EA
Steam Production Rate	2 kg/s
Heater Power	2 MW
Power used for SOEC	25 MW
Hydrogen Tank Pressure	20 bar
Hydrogen Production Rate	13 tonnes/day
Electricity Required	46.56 kWh _e /kg-H ₂

ACKNOWLEDGEMENT

This work is supported by the Nuclear Research & Development program in the form of a National Research Foundation (NRF) grant funded by the Korean government Ministry of Trade, Industry, and Energy (No. 2021M2D1A1084837).

REFERENCES

- [1] Konor Frick, Paul Talbot, Daniel Wendt, Richard Boardman, Cristian Rabiti, Shannon Bragg-Sitton (INL) Evaluation of Hydrogen Production Feasibility for a Light Water Reactor in the Midwest, September 2019
- [2] Keon Yeop Kim, Youngsuk Bang, So Eun Shin, Jung Jin Bang "Coupling Analysis of SMART100 for Thermal Energy Extraction" Transactions of the Korean Nuclear Society Autumn Meeting Changwon, Korea, October 20-21, 2022
- [3] KHNP, KAERI, KACARE, SMART100 Standard Safety Analysis Report, 2019.
- [4] P. Fritzon, OpenModelica User's Guide Release v1.19.0-dev-107-g6ac89ac5ea9, Open Source Modelica Consortium, 2021.

[5] Meng Li, Michael K.H.Leung, Dennis Y.C.Leung, An Electrochemical Model of a SolidOxide Steam Electrolyzer for Hydrogen Production, Chem. Eng. Technol. 29, No.5, (2006).

[6] Meng Li, Michael K.H.Leung, Dennis Y.C.Leung, Parametric Study of Solid Oxide Steam Electrolyzer for Hydrogen Production, International Journal of Hydrogen Energy 32, (2007).

[7] Daniel S Wendt, Lane T Knighton, High Temperature Steam Electrolysis Process Performance and Cost Estimates - DOE Hydrogen Program AMR Presentation, June, 2022 (INL)