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TECHNOLOGY BRIEF

MODELING THE FLEXIBLE OPERATION OF ELECTROLYZERS FOR HYDROGEN PRODUCTION IN A LOW-CARBON ENERGY SYSTEM

Important Considerations

THE RESEARCH FRAMING

In a future low carbon energy system, flexible assets such as electrolyzers could be deployed to increase the uptake of variable renewable energy (VRE) on the grid and to utilize available renewable energy sources more efficiently. An understanding of the technical and economic factors with VRE use and hydrogen production in electrolyzers need to align across electricity supply, hydrogen production, and hydrogen offtake/use.

THE VALUE

Hydrogen's role in the changing energy landscape is yet to be determined and could vary significantly across investors, utilities, vendors, and end users. Modeling electrolyzers, especially at a systems scale, is crucial to understanding how they can be optimized for overall hydrogen production.

LCRI'S FOCUS

Research is needed to investigate the effect of variations in temporal and spatial resolutions of variables (O&M costs and electrical current availabilty) on the total hydrogen production in electrolyzers. This would help stakeholders make best use of their available assets while minimizing the cost of hydrogen production from electrolyzers.

INTRODUCTION

Wind and solar electricity are increasingly deployed worldwide as part of efforts to reduce consumer costs and support decarbonization targets. These renewable energy resources are typically characterized by low-capacity factors (between 25% and 51%) and generation profiles that do not match grid electrical load demands [1,2]. To increase the uptake of variable renewable energy (VRE) on the grid and to more efficiently utilize available renewable energy sources, electrolyzers could be deployed as flexible assets. However, technical and economic factors need to align across electricity supply, hydrogen production, and hydrogen offtake/use.

Flexibility in the power system can be characterized by the system's ability to respond to changes in electricity supply and demand [3]. Increased VRE penetration in the electrical grid induces uncertainty in the security of supply [4]. Furthermore, flexibility and grid-balancing requirements are needed at all time scales and could range from short-term frequency regulation to long-term resource adequacy measures. Seasonal variation in VRE supply could also lead to requirements for longer-duration energy storage when fossil fuels with CO_2 abatement are not available or deployed [5].

A scenario-based analysis conducted using the United States Regional Economy, Greenhouse Gas, and Energy (US-REGEN) model[1] shows energy storage (chemical, electrochemical, mechanical, and thermal energy-storage technologies) plays a more significant role in deep decarbonization when fossil generation is not deployed (i.e., when CO_2 capture, removal, or negative-emission technologies are not deployed with fossil fuels). In scenarios where the share of VRE in electricity supply increases to approximately 70% and fossil generation becomes unavailable, energy storage becomes more competitive for balancing renewables. These scenarios show that hydrogen-fired power generation and energy-storage discharge provide about 9% of the total electricity supply for end uses in the United States. At 100% renewables, energy storage becomes even more important, with hydrogen-fired generation and energy-storage discharge providing 108 TWh and 627 TWh respectively, which constitutes about 20% of total electricity supply for end uses [6].

Electrolyzers could provide an energy system with flexibility while helping to balance an electric grid with high penetration of VRE resources. Understanding grid-balancing requirements (e.g., peak shaving and frequency regulation) along with electrolysis technology limitations and potential (e.g., electrolyzer response rate and electrolyzer efficiency) is crucial to understanding electrolyzers' place in a low-carbon landscape. Operational modes and deployment strategies affect electrolyzer efficiency and durability, which impact hydrogen-production economics. Combining energy systems' economic models with electrolyzer technology models could enable a deeper understanding of scenario-specific electrolyzer applications. Various stakeholders, including technology investors, electric utilities, and hydrogen end users, could use the combined models to address the following:

- Hydrogen production that maximizes grid operations
- Conditions for siting and sizing electrolyzers for optimal hydrogen production
- Operational performance and system efficiencies for various electrolyzer and grid profiles

An expanding VRE portfolio in many countries calls for resourceful interactions between the electricity provider and the electrolyzer equipment provider, which may benefit both parties while proving economical for hydrogen customers. The mode of operating an electrolyzer could vary significantly depending on whether the electrolyzer operator is an electricity provider, grid operator, technology investor, or hydrogen producer, because each type of operator would define the profitability of using an electrolyzer differently. For instance, an electricity provider could operate the electrolyzer in a manner that maximizes renewable electricity's capacity factor while minimizing curtailment. In another example, a transmission system operator could prioritize electricity use for short- and long-term supply security. In this scenario, electrolyzers could simply be used as capacity reserves, where capacity payments in some cases have been estimated to be as high as \$20–30/kW-month [5].

Another benefit of electrolyzers is sector coupling with renewable electricity. Sector coupling refers to integrating different sectors across the energy system (e.g., power-to-gas that integrates the electricity supply side with the gas sector). Sector coupling using electrolysis-produced hydrogen could enable medium- to large-scale reserves, reduce curtailment, and act as an additional energy vector for supply security. An electrolyzer operator considering hydrogen production for industrial applications may prioritize locating the electrolyzer to be able to continuously run the electrolyzer and maximize inexpensive electricity availability, or the operator may prefer a load-following electrolyzer to maximize renewable electricity

1 Details on US-REGEN can be found at https://us-regen-docs.epri.com.

utilization. Lowering hydrogen production cost while optimizing case-specific results requires understanding the breakdown of how electrolyzer costs that contribute to hydrogen-production economics are balanced against operational considerations, broad grid conditions, and hydrogen demand.

One of the main costs involved in hydrogen production from electrolyzers at present is the capital cost of the main system components, but other costs could become dominant as the market matures [7]. Many vendors are targeting lower capital costs by expanding manufacturing capabilities and achieving economies of scale. Many are also working toward lower operation and maintenance (O&M) costs, higher system efficiencies, and improved reliability and availability. Hence, a common and coordinated understanding of the integration, operation, and optimization of the various energy vectors' demand, supply, and costs has become essential when integrating electrolyzer equipment with the electric grid and offtakes in other sectors [8]. Although lower capital costs depend more on vendor pricing, the operator has some control in keeping O&M costs low. An electric grid operator choosing to operate flexibly may benefit from operating electrolyzers only during periods of low electricity cost, whereas an end-use operator could benefit from baseload, high-capacity operation, with electrolyzer siting and sizing playing a more significant role. Identifying critical electricity system parameters and integrating them with electrolyzer operating models when connecting the upstream and downstream electrolyzer processes is crucial to ensuring efficient and reliable transformation toward renewable energy.

UNDERSTANDING ELECTROLYZER MODELING

Types of Electrolyzers and Their Parts

Electrolyzers can be classified based on their operating temperatures, charge carriers, and electrolytic materials. Typically, electrolyzers operating within 68 to 212°F (20 to 100°C) [9,10] are classified as low-temperature electrolyzers (LTE), and electrolyzers operating within 1382 to 1832°F (750 to 1000°C) [11] are classified as high-temperature electrolyzers (HTE). Theoretically, the following five types of electrolyzers can be identified based on the three defining factors:

- LTE, alkaline electrolysis with OH^- ion carrier
- LTE, solid polymer electrolyte with OH^- ion carrier, commonly known as anion exchange membrane (AEM) electrolysis
- LTE, polymer electrolyte membrane (PEM) with proton ion charge carrier
- HTE, solid oxide electrolytic membrane with proton ion charge carrier
- HTE, solid oxide electrolytic membrane (SOEC) with oxide ion charge carrier

These electrolysis technologies are at varying maturity levels and have the potential to provide value in producing renewable hydrogen for different purposes [11]. Modeling electrolyzer systems based on their specific stack and system parameters (see Table 1) is useful for optimizing the energy system performance under different operational conditions of temperature, pressure, and electrical current availability.

Identifying the types of electrolyzers is necessary to define technology-based operational considerations. Due to their low response times, LTEs are typically more suitable for maximizing hydrogen production for a load-following electrical current profile. With their higher overall efficiency, HTEs have the potential to produce more hydrogen than LTEs do for the same energy consumption at baseload operation [12]. However, the optimal operational mode and technology requirement could vary based on case-specific considerations and electricity cost.

Understanding the physical variables that affect overall hydrogen-production capabilities is important when considering modeling pathways for electrolyzers. Table 1 lists parameters on which hydrogen production from an electrolyzer depends. These parameters have been identified based on past scientific studies and physical representations of electrolyzers in the form of electrochemical, thermochemical, and fluidic equations. When modeling an electrolyzer, understanding these parameters' variability aids in accurately representing the electrolyzer's operation.

Table 1: Technology-specific parameters that influence electrolyzers' overall renewable hydrogen production [13]

Electrolyzer System Parameters	Stack and Membrane Parameters	Process Parameters
Stack cell voltage	Operating temperature	Ambient temperature
Maximum current density	Operating pressure	Electrical current availability
Minimum current density	Thermal response time	Total water consumption
Efficiency	Diameter of cells	
Hydrogen production	Number of cells	
Required oxygen purity	Conductivity/resistance of cells	
Required hydrogen purity	Surface area of cells	
Required final hydrogen pressure	Anode resistance	
Activation energy at anode	Cathode resistance	
Activation energy at cathode	Membrane thickness	
System heating and cooling requirement	Membrane porosity	
	Permeability for H_2	
	Permeability for O_2	

Electrolyzer Modeling Domains

Modeling electrolyzers from an energy system perspective could help in estimating a system's energy, mass, and heat flows. This modeling can also help with planning resources to understand and optimize operation of the electrolyzer to maximize hydrogen production. To date, much scientific literature has been published on modeling electrolyzers.

To model the various processes inside an electrolyzer, the following five domains are considered:

- Electrical – Connecting the electrical components from the grid to the electrolyzer. This includes rectifiers and transformers.
- Thermal – Mapping changes in the operational temperature inside the cell. These changes can influence efficiency and hence energy-related hydrogen production in the electrolyzer.
- Electrochemical – Accounting for the electrical energy required to break the chemical bonds in the water molecule. Different types of electrolyzers have different ion carriers and hence different thermodynamics related to water splitting, and could aid in understanding stack mechanisms and efficiency.
- Fluidic – Mapping the fluid dynamic motion of liquids and gases inside the electrolyzer.
- Thermochemical – Accounting for the thermal changes on the chemical bonds and molecule splitting inside the electrolyzer.

After the domains in the electrolyzer have been identified, the modeling approach is identified [14,15]. An electrolyzer model requires the following three considerations:

- Model type
- Model dimensionality
- Model state

Model Type

A. **Empirical/semiempirical models** use parametric equations obtained by mathematically equating experimental curves. Empirical equations are not necessarily mathematically or physically consistent and could differ for various electrolyzer types. Semi-empirical equations combine the use of empirical equations with some physical models. Although empirical and semi-empirical model equations are repeatable and relatively less complex, they are usually specific to only a certain type of electrolyzer and do not allow for scaling studies.

B. **Analytical models** are based on physical law equations. Modeling using these equations provides a theoretical representation of an electrolyzer stack and system. Analytical equations represent a simplified version of a mechanistic model.

C. **Mechanistic models** draw on the laws of physics and electrochemistry. The equation inputs differ based on the characteristics of the electrolytic cell, stack, and system.

Once the type of model description has been established, the model can be described at a cell level or a system level. The model dimensionality could be zero cell dimensional, or 0-D (i.e., all cells in the stack are assumed to have the same response to the electrical signal), or the model could include up to three spatial dimensions, where the length, breadth, and width of the system design could be considered.

Model dimensionality

A. **Cell/stack (0-D)** considers only one cell in most of the models reviewed, based on the assumption that all cells behave in the same way. Hence, stack variables are computed based on cell variables and the number of cells.

B. **System (1-D to 3-D)** includes the balance-of-plant and auxiliaries. These models consider temporal and spatial resolutions of electrolyzer systems.

The models developed can be used to describe the electrochemical and thermochemical domains inside the electrolyzers, which could be static (steady) or dynamic.

Model state

A. **Static or steady-state models** are based on algebraic equations between the variables of the model that do not include time: x = f (y).

B. **Lumped-parameters dynamic models** are given by ordinary differential equations (ODE): the behavior depends on time. This easy-to-resolve model type, called an "input-output model," is typically used for system control analysis.

C. **Distributed-parameters dynamic models** are represented by partial differential equations (PDE): the behavior depends on time and space. The models (complex and resolved using finite elements) are used mainly for sizing, chemical and thermal process design, and analysis.

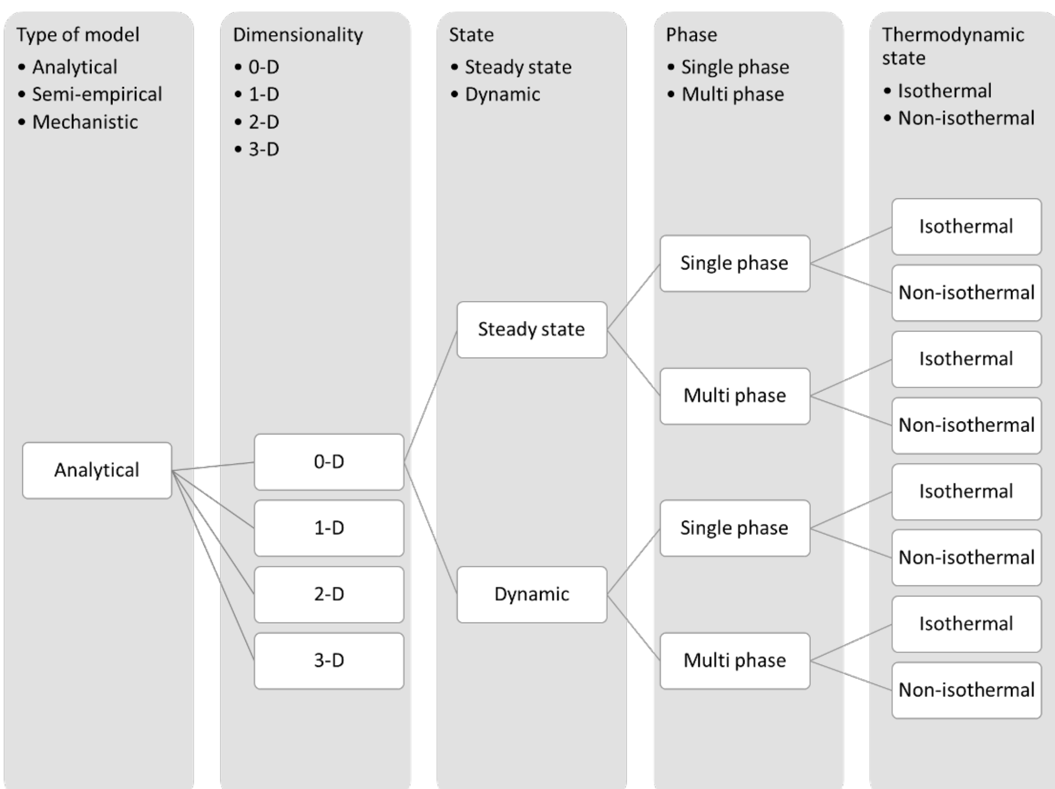


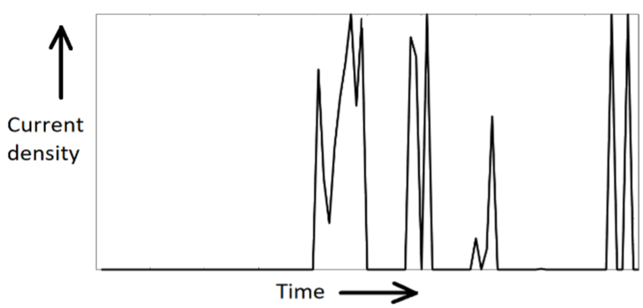
Figure 1: Pathways to modeling an electrolyzer's domains, with an example of a modeling pathway.

In addition to the factors above, single-phase or multi-phase equations with isothermal or non-isothermal conditions can be considered, depending on the complexity level (see Figure 1).

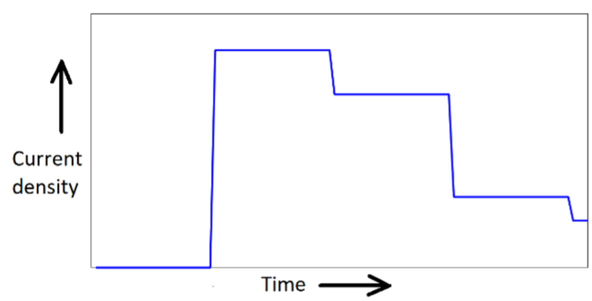
Existing electrolyzer models have commonly followed mechanistic and semi-empirical approaches to modeling an electrolyzer [16–26]. Both approaches require inputs from an actual electrolyzer. Although semi-empirical models used in Dale (2008) and Santarelli (2009) can aid in much more accurately representing the cell and stack parameters [16,17], the models would need continuous feedback from the specific electrolyzer. However, changes in the system (i.e., changes in temperature and flexible loads for that specific electrolyzer) need technology- and input-specific results, as opposed to changes in an energy system, where the electrolyzer inputs could be variables. Mechanistic model approaches used in Onda (2002), Choi (2004), Gorgun (2006), Marangio (2009), Grigoriev (2009), Awasthi (2011), Lee (2013), Nie (2010), and Kim (2013) show detailed equations from all electrolyzer domains [18–26]. Choi (2004) shows that the overpotentials at the anode and cathode have a significant effect on the electrolyzer's overall inefficiencies [19]. Hence, analytical equations focusing on major regions of inefficiencies and building up to a detailed mechanistic model approach would aid in developing an input-driven electrolyzer systems model.

At present, the energy landscape is changing significantly toward increased VRE utilization. Using an input-driven analytical approach to modeling electrolyzers would aid in adapting electrolyzer models to different scenarios. Table 2 summarizes the results from a study that uses an analytical approach with 0-D dynamic modeling in a single-phase, non-isothermal model [12]. Here, total curtailed electricity is summarized in three different ways to represent an electrolyzer's potential operational modes (see Figure 2 a-c). The results are summarized as the deviation in total hydrogen production from a base case for a PEM and SOEC electrolyzer model.

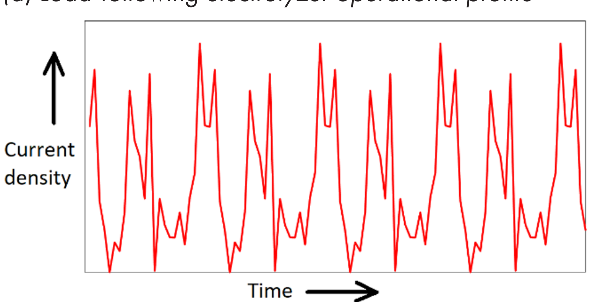
The case study results show that the maximum deviation in total hydrogen production for a low-temperature operation PEM electrolyzer is 7.7%, whereas the maximum deviation is almost 66% for a high-temperature SOEC. This shows that an HTE may not be suitable for flexible operation in this scenario. Although the PEM electrolyzer itself shows the least hydrogen production for a load-following profile, it is the better option when compared to SOEC, for which potential hydrogen-production deviation from baseload could be as high as 66%. This approach can aid decision makers considering scenarios in which the electrolyzer technology cannot be operated at baseload.



(a) Load-following electrolyzer operational profile



(b) Daily average electrolyzer operational profile



(c) Monthly average operational profile

Figure 2: Potential operational modes of electrolyzers coupled with VRE [12].

Table 2: Effect of low- and high-temperature electrolyzers' various operational modes on the deviation in total hydrogen production from baseload operation [12]

Technology	**Deviation in Total Hydrogen Production from Baseload Operation**		
	Figure 2(a)	**Figure 2(b)**	**Figure 2(c)**
PEM	-7.71%	-3.3%	-2.64%
SOEC	-65.66%	-29.31%	-46.23%

CONCLUSIONS

Factors such as electrolyzer type (technology based), electrical current profile (grid based), and end-use factors can affect electrolyzers' overall hydrogen production. Scenario building for electrolyzers in the present or for a future energy system could include supply-side considerations, technology-based considerations, or both. These considerations would aid in determining the electrolyzer's operational mode. Hydrogen's role in the changing energy landscape is yet to be determined and could vary significantly across investors, utilities, vendors, and end users. Modeling electrolyzers, especially at a systems scale, is crucial to understanding how they can be optimized for overall hydrogen production.

The analysis of the results from Table 2 indicates that statistical analysis of electrolyzers' operational modes is needed to fully understand how hydrogen production can be maximized for different technologies and use cases. For example, a utility considering a load-following application to maximize VRE utilization may benefit from an LTE because it shows reduced hydrogen-production losses compared to an HTE. However, an investor in an HTE that operates their electrolyzer flexibly might want to minimize operational variations to minimize hydrogen-production losses. Operating an HTE with daily averages (Figure 2b) shows the least deviation in hydrogen-production potential. An end user with access to low-cost electricity and potential offtake may consider operating an HTE as much as possible to maximize hydrogen production.

Electrolyzers are at present an expensive technology, and deeper understanding of the case-based optimized operational mode would aid investors in understanding how to maximize return on their investments. Deciding how and when to operate an electrolyzer would be influenced by the availability of low-cost electricity and water, in addition to the hydrogen-production site's proximity to the offtake. Future studies that investigate combining hydrogen-production optimization with additional factors would aid decision makers, utilities, vendors, and end users in making best use of their available assets, while minimizing the cost of hydrogen production from electrolyzers.

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