Systems & Control Transactions

Research Article - Peer Reviewed Conference Proceeding
ESCAPE 35 - European Symposium on Computer Aided Process Engineering
Ghent, Belgium. 6-9 July 2025
Jan F.M. Van Impe, Grégoire Léonard, Satyajeet S. Bhonsale, Monika E. Polańska, Filip Logist (Eds.)

PSE PRESS

Development of a hybrid, semi-parametric Simulation Model of an AEM Electrolysis Stack Unit for large-scale System Simulations

Isabell Viedt[a,c]*, Michel Große (né Mock)[a,c], and Leon Urbas[a,b,c]

[a] Technische Universität Dresden, Process-to-Order Group, Process Systems Engineering Group
[b] Technische Universität Dresden, Process-to-Order Group, Chair of Process Control Systems
[c] Technische Universität Dresden, Process-to-Order Group, Process-to-Order (P2O) Lab Learning Factory
* Corresponding Author: isabell.viedt@tu-dresden.de.

ABSTRACT

A key technology for integrating fluctuating renewable energy into the process industry is the production of green hydrogen through water electrolysis plants. Scaling up electrolysis plant capacity remains a significant challenge for the renewable energy transition. System simulation of large-scale electrolysis plants can support process design, monitoring, optimization, and maintenance scheduling. Hybrid modeling methods are promising for improving simulation reliability by combining process knowledge with process data, addressing gaps in understanding of the underlying processes. These hybrid, semi-parametric models have shown improved accuracy than purely mechanistic models. This study develops a hybrid, semi-parametric model for an anion exchange membrane electrolysis (AEMEL) stack unit. Parameters such as heat loss and heat transfer, which cannot be directly measured, are estimated using real process data. Sensors provide data on lye tank temperature, outlet temperature, and flow rate, enabling estimation of heat transfer coefficients and losses. The hybrid model is validated against operational data from different load settings of the AEMEL stack unit. To test its scalability, a large-scale electrolysis plant configuration is simulated, comprising multiple AEMEL stack units, a water supply module. Performance accuracy and efficiency of the hybrid model are compared with the mechanistic model. This hybrid model lays the foundation for future use in efficient system simulations with surrogate models, potentially enhancing large-scale electrolysis plant performance and renewable energy integration.

Keywords: Hydrogen, Modelling and Simulations, System Simulation, Hybrid Modeling, Modular Plants

INTRODUCTION & BACKGROUND

A crucial technology for integrating variable renewable energy into the process industry is the production of green hydrogen through water electrolysis. Scaling-up electrolysis plant capacity remains a significant challenge in facilitating a successful transition to renewable energy. One potential pathway to successfully scale-up the hydrogen production is the numbering-up of electrolyzer systems using modular plant concepts, according to VDI 2776 [1]. This approach allows for the combination of different electrolysis technologies and electrolyzer scales within one process plant a so-called modular, heterogeneous electrolysis to achieve higher flexibility of start-up, shut-down and operation [2].

With this, the system simulation of these large-scale electrolysis plants can be utilized for process design but also for process monitoring and optimization, and maintenance scheduling [3]. Since the underlying processes for the simulation models are often not completely understood, hybrid modeling methods are a promising approach to combine process knowledge with process data for more reliable and precise simulation models [4]. These hybrid, semi-parametric models

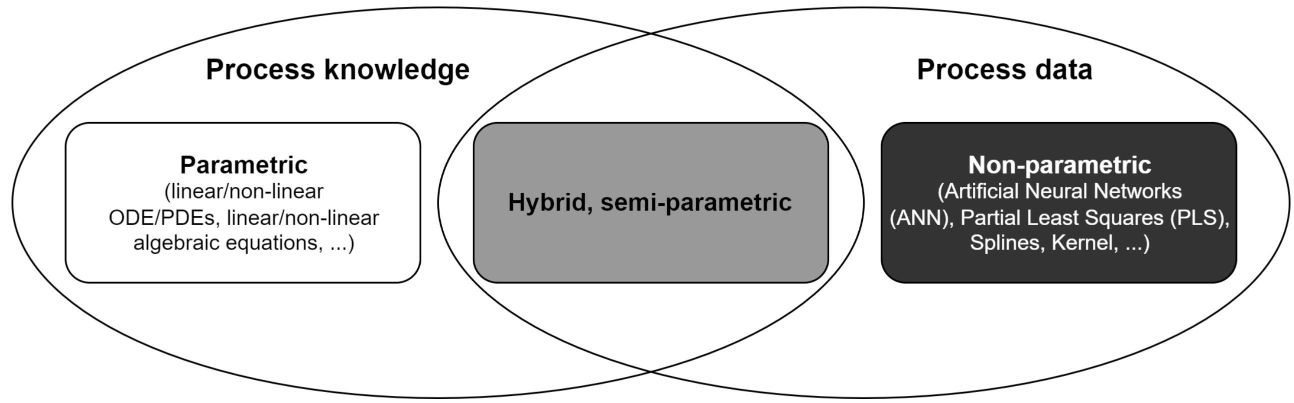

Figure 1. Taxonomy of hybrid, semi-parametric models.

achieved better accuracy and prediction quality than knowledge-driven mechanistic models.

In this work a hybrid, semi-parametric model for an anion exchange membrane electrolysis (AEMEL) stack unit is developed. The basis of this model is a mechanistic model of the AEMEL stack unit [5]. To evaluate the applicability of the hybrid, semi-parametric AEMEL model within a large-scale system simulation context, an electrolysis plant configuration is designed including multiple AEMEL stack modules, a water supply module and post-processing steps for the produced hydrogen. This plant configuration is then simulated using both the hybrid, semi-parametric and mechanistic AEMEL models to compare performance accuracy and simulation efficiency of both model types. In future work, this hybrid, semi-parametric model could be the basis for creating more efficient system simulations utilizing surrogate models.

METHODOLOGY

Modeling for flexible, heterogenous water electrolysis plants

Simulation models of entire process chains can be used to evaluate plant structures and provide virtual testing capabilities of developed automation and control concepts [6,7]. With the scale-up of water electrolysis plants following modular standards [2], the modeling approach must also follow this approach [3,8].

In the research project eModule this modular, flexible modeling approach is followed to investigate the applicability and operability of these modular heterogenous water electrolysis plants. The project aims to develop open-source model repositories. Dynamic stack unit models were designed for low-temperature electrolysis technologies, namely alkaline electrolysis (AEL), proton exchange membrane electrolysis (PEMEL), as well as anion exchange membrane electrolysis (AEMEL) [5]. Further dynamic models for the balance of plant (BoP) components like e.g., lye circulation and water supply were designed [3,8]. Additionally, a dynamic partial model for solid-oxide high-temperature electrolysis (SOEL/HTEL) was developed as a black-box model [9]. Details on the developed models can be found in [5] and the linked Github repository in the supplementary material.

To ensure accurate estimation and system simulation, process data is used to refine and validate the simulation models resulting in more accurate hybrid, semi-parametric simulation models as compared to the currently existing mechanistic models.

Hybrid, semi-parametric modeling

Mechanistic models form a broad and transparent class, typically based on fundamental principles such as conservation laws [4]. In contrast, data-driven models rely solely on process data, offering a less transparent modeling approach [10].

Hybrid semi-parametric models, also known as gray-box models, integrate parametric and non-parametric sub-models derived from different knowledge sources. These models offer several advantages over traditional mechanistic or purely data-driven approaches [11]. An overview of hybrid semi-parametric simulation models is presented in Figure 1. Key benefits include a broader knowledge base, greater transparency in modeling, and cost-effective development [10]. In complex process simulations, hybrid approaches provide more accurate and robust estimations [11,12]. Gray-box models leverage existing process data through machine learning (ML) or artificial intelligence (AI) algorithms, effectively bridging gaps in mechanistic modeling [10].

CASE STUDY

The presented case study covers the applicability and performance evaluation of gray-box models e.g., hybrid, semi-parametric simulations models, within system simulations of large-scale, modular water electrolysis plants.

Anion Exchange Membrane Electrolysis

The Anion Exchange Membrane Electrolysis (AEMEL) is a low-temperature technology that combines advantages of PEMEL and AEL: operational flexibility (PEMEL) and low investment and operational costs (AEL) [13]. Currently, three AEMEL stack units, combined into one AEMEL module, exist as a demonstrator within the module pool of the Process-to-Order (P2O) Lab Learning Factory at TU Dresden.

The base level model for the hybrid, semi-parametric AEMEL stack model is a mechanistic AEMEL stack model developed in MATLAB/Simulink, modeled according to generic modular modeling principles [5]. Dimensionality is neglected for the base model since high computational power is required for 1D – 3D models and does not align with the goal of modular system design and automation. Therefore, the model is constructed as a lumped parameter (0D) model. To develop a lumped simulation model of the electrolyzer stacks, each cell side—anode and cathode—is represented as an ideal continuously stirred tank reactor (CSTR), with the separator or membrane serving as a shared interface.

To ensure a generic stack-unit model, first-principles models are prioritized, with the option to extend them using customizable empirical equations [5]. Several submodels, namely the mass accumulation/transfer, thermal, fluidic, electrochemical, and electric models, are each considered. Equations (1) – (6) show the generic mass accumulation/transfer submodel and the generic energy accumulation and thermal submodel as they are the most relevant for the hybrid, semi-parametric modeling part in the next section. Further model equations and assumptions can be found in [5].

The mass accumulation is modeled as dynamic component mass balances for each component i in each cell side j, according to (1):

$$\frac{dm_i^j}{dt} = \dot{m}_{in}^j \omega_{in,i} - \dot{m}_{out}^j \omega_i^j + \dot{m}_{R,i}^j \pm \dot{m}_{cross,i} \quad (1)$$

with $\dot{m}_{in}^j$ as the inlet mass flow in each cell side, $\omega_{in,i}$ as the inlet mass fraction of each component, $\dot{m}_{out}^j$ out as the outlet mass flow in each cell side, ω_i^j as the mass fraction of each component in each cell side, $\dot{m}_{R,i}^j$ as the reaction rate (cf. equation 2) of each component in each cell side and $\dot{m}_{cross,i}$ as the crossover flow through the common interface.

The thermal model determines the temperature within the stack unit, which is crucial for calculating thermo-physical substance properties and cell voltage. Cell temperatures are computed using dynamic energy balances for each cell side, as described in equation (2):

$$\frac{dE^j}{dt} = \dot{m}_{in}^j e_{in} - \dot{m}_{out}^j e^j \pm \dot{m}_{cross} e^j + \dot{Q}_{loss} - \dot{Q}_{amb} - \dot{Q}_{hx} \quad (2)$$

with $\dot{Q}_{loss}$ as the heat generated due to current losses in the reaction, $\dot{Q}_{amb}$ as the heat exchanged with the surrounding environment and $\dot{Q}_{hx}$ as heat exchanged between the cell sides due to temperature difference.

$$\dot{Q}_{loss} = i\, A_{act}(U_{cell} - U_{tn}) \quad (3)$$

U_{cell} is the voltage of the electrolytic cell and U_{tn} the thermoneutral voltage of the water electrolysis reaction described by equation (4) with ΔH as the reaction enthalpy at operating conditions.

$$U_{tn} = \frac{\Delta H}{n\, F} \quad (4)$$

The heat exchange $\dot{Q}_{amb}$ with the environment is calculated for both cell sides according to (5) [14]:

$$\dot{Q}_{amb} = k_{amb} A_{amb} (T^j - T_{amb}) \quad (5)$$

with k_{amb} as the heat transfer coefficient from the stack unit to the environment, A_{amb} as half the surface area of the stack, due to the heat loss occurring in both cell sides, and T_{amb} as the assumed constant ambient temperature. Similarly, the internal heat exchange between the cell sides is modeled according to (6):

$$\dot{Q}_{hx} = k_{hx} A_{hx} (T^{an} - T^{cat}) \quad (6)$$

with k_{hx} as the heat transfer coefficient between the cell sides, A_{hx} as the heat exchange area inside the stack unit and $T^{an/cat}$ as the respective temperatures inside the anode and cathode channel. The coefficients for k_{amb} and k_{hx} can be determined based on the prevailing flow regime and cell structure, derived empirically for specific stack units, or assumed constant [15]. In case of this generic modeling approach, constant values are assumed.

To enhance flexibility and reusability, the model interfaces are designed to be compatible with advanced mass and energy balance frameworks commonly used in flowsheeting tools. Additionally, the developed models are exported as Functional Mock-Up Units (FMUs), allowing for platform-independent model exchange [5].

Hybrid AEM Model

The model parameters for the current mechanistic AEMEL model are based on literature estimations [16-18] and do not fully represent the existing lab setup (cf. [5]). The AEMEL was purchased as a pre-configured stack unit by Enapter. It offers a limited number of sensors for process data collection and cannot be retrofitted.

The heat loss within stack, pump, heat exchanger and piping cannot directly be measured and therefore must be approximated through non-parametric estimation from process data. In addition to hydrogen output $\dot{m}_{H_2,out}$, available sensors collect data for the temperature in the lye storage tank T_{tank}, the outlet temperature of the stack-unit $T_{out,1}$ and the flow rate into the stack $\dot{m}_{lye,out}$. Using the available data and the mechanistic stack model, the heat loss $\dot{Q}_{amb}$ to the environment defined by k_{amb} can be estimated.

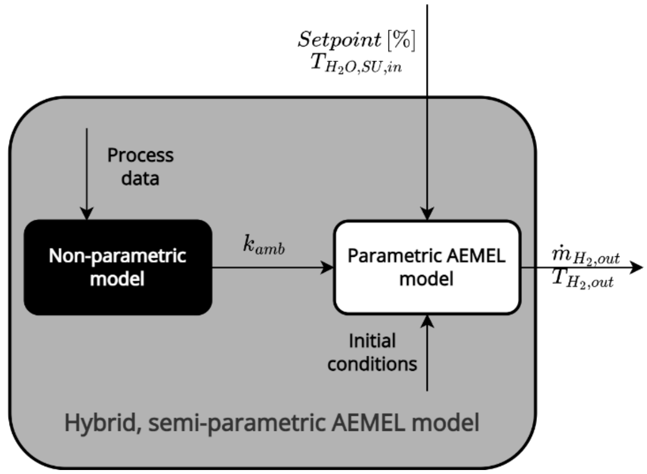

Figure 2. Structure overview of the hybrid, semi-parametric AEMEL stack unit model.

The hybrid, semi-parametric model was developed in MATLAB/Simulink as a light gray-box model. The model structure is shown in Figure 2. Currently, the data utilized for the non-parametric estimation within the hybrid model is synthetic process data. The load setpoint of the stack unit and the inlet water temperature $T_{H_2O,SU,in}$ were identified as the control parameters for the AEMEL. To emulate the behavior or real process data collected from the plant, random noise was added to the generated synthetic data from the simulation. The random noise is related to the maximum value of each batch run and simulation output. The Design of Experiments for the data generation is shown in Table 1.

Table 1: Design of Experiments (DoE) for the control parameters for synthetic data generation.

Control Parameter	*Load Setpoint* [%]			$T_{H_2O,SU,in}$ [°C]		
Value	33	66	100	5	25	45

Setup of the System Simulation

The goal of the generic modeling approach for flexible, heterogenous water electrolysis plants is to aid scale-up design and the optimization of plant operation to accommodate price-driven hydrogen production utilizing fluctuating, renewable energy [3]. Therefore, the developed simulation models are tested for their applicability and performance in medium- and large-scale system simulations. The performance of the hybrid, semi-parametric model within the system simulation is compared to the performance of the mechanistic model.

The configuration of the evaluated system simulation is shown in Figure 3. The simulation represents a medium-scale, homogenous electrolysis system which includes 18 AEMEL Stack Units, one Water Supply Unit and Distribution and Mixing Units for the material streams. For the AEMEL, three stack units are aggregated into one module unit, which reflects the laboratory setup for the M16 module in the P2O Lab Learning Factory. The nominal system size is 43.2 kW.

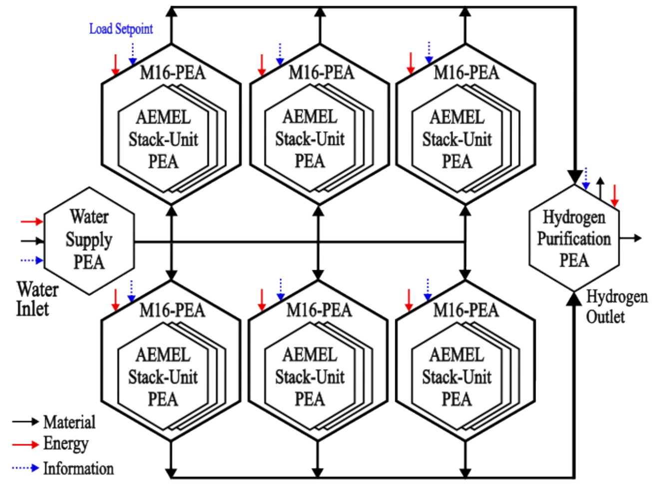

Figure 3. Modular plant layout for the presented system simulation with AEMEL.

The system simulation is set up in MATLAB/Simulink as a co-simulation environment shown in Figure 3. To evaluate the applicability of the hybrid, semi-parametric AEMEL model, a load input scenario into the system covering one day of solar power production was selected. The simulation scenario represents the load input for one day of solar power into the electrolysis plant with the input in 5-minute time-steps. The specifications for the simulation scenario can be found in [19]. The simulated system follows the requested load changes of the solar power input profile to emulate real price-driven plant operation.

Performance Evaluation & Discussion

The performance of the hybrid, semi-parametric AEMEL stack unit model was compared to the previously developed mechanistic AEMEL stack unit model within a system simulation. A comparison of the simulation results for the solar power scenario is shown in Figure 4.

The results show that both the mechanistic and the gray-box system simulation are able to follow the flexible solar power profile with the hydrogen production rate $\dot{m}_{H_2O,plant}$. As shown in Figure 4 (right), the behavior of the hybrid model differs significantly in the temperature profile. The non-parametrically estimated value for k_{amb}

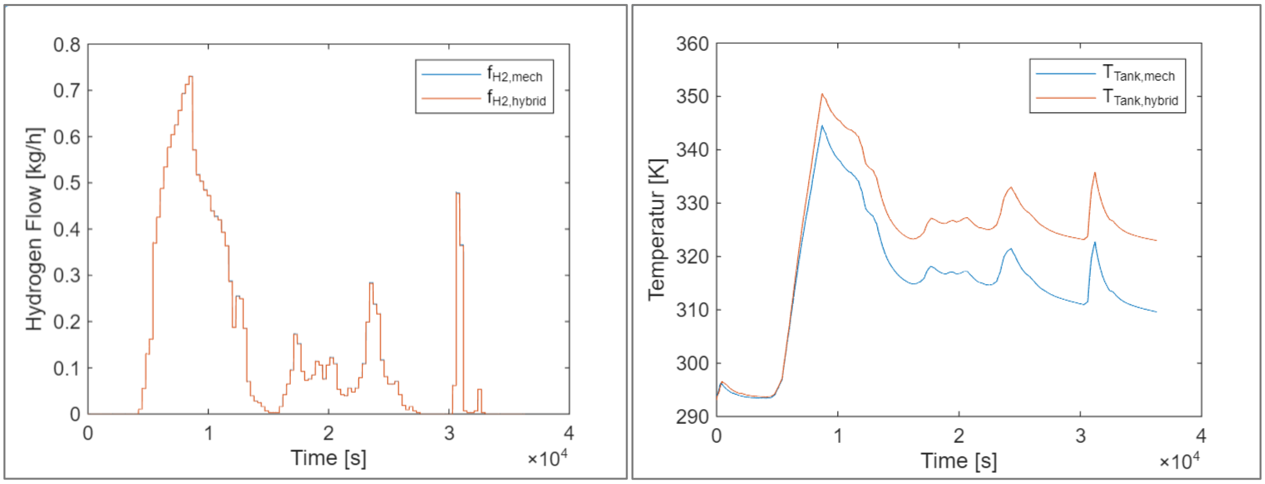

Figure 4. Comparison of simulation results for the system simulation: overall hydrogen production rate (left) and stack outlet temperature (right).

is lower than the originally defined value within the mechanistic model. Therefore, the overall heat loss from the system to the environment was overestimated and model reaches a higher temperature in the stack.

Due to the utilization of the synthetic process data for model development, the behavior of the hybrid, semi-parametric AEMEL model resembles the very detailed mechanistic model closely. This problem be amended once real process data can be collected from the demonstrator plant. One approach to leveraging this would be the utilization of more complex physics-informed neural networks (PINNs) [20].

Conceptually, gray-box models, not just hybrid, semi-parametric models, can be utilized in different real-time plant operation scenarios. Especially, in flexible, modular electrolysis plants, which are designed to follow fluctuating power input profiles [7,21], hybrid model structures that utilize online process data allow faster adaption to partial load production and more accurate forecasting of ramp-up and ramp-down cycles.

CONCLUSION AND OUTLOOK

The presented case study verified the applicability of hybrid models within system simulation of modular water electrolysis systems. Currently, the significance and impact value of the developed hybrid, semi-parametric AEMEL model is limited as the model was developed using only synthetic process data. This represents the first step in the refinement of the generic simulation models for the modular water electrolysis concept. This paper builds the foundation for the concept development of a hybrid, semi-parametric simulation model pool as an addition to the already existing model pool.

A next step in the system simulation for electrolysis scale-up could be the development of faster and less computationally intensive surrogate models from the more accurate hybrid, semi-parametric simulation models. The surrogate models can further be utilized to setup more sophisticated Digital Twins to be used for real-time monitoring and optimization during plant operation.

DIGITAL SUPPLEMENTARY MATERIAL

The P2O-Lab Learning Factory provides a Github group repository which contains the individual model repositories of the developed simulation models for the generic modular electrolysis plant. It is currently only available upon individual request at https://github.com/orgs/p2o-lab/teams/ap2_external/repositories. The repository includes the mechanistic and hybrid AEMEL stack unit models which are evaluated in this paper. It also provides the models for the balance of plant components and the other electrolysis technologies. The repositories will be openly accessible starting from October 2025.

ACKNOWLEDGEMENTS

We would like to thank the German Federal Ministry of Education and Research and the project management organization Jülich for their financial support within the framework of the eModule research project (FKZ 03HY116A) of the H2Giga lead platform.

REFERENCES

1. VDI 2776 Blatt 1, Process engineering plants - Modular plants - Fundamentals and planning modular plants. 2020. Accessed: Apr. 29, 2022. [Online]. Available: https://www.vdi.de/richtlinien/details/vdi-2776-

blatt-1-process-engineering-plants-modular-plants-fundamentals-and-planning-modular-plants
2. Lange, H., Klose, A., Beisswenger, L., Erdmann, D., & Urbas, L. (2024). Modularization approach for large-scale electrolysis systems: a review. Sustainable Energy & Fuels.
3. Mock, M., Viedt, I., Lange, H., & Urbas, L. (2024). Heterogenous electrolysis plants as enabler of efficient and flexible Power-to-X value chains. In Computer Aided Chemical Engineering (Vol. 53, pp. 1885-1890). Elsevier. doi: 10.1016/B978-0-443-28824-1.50315-X.
4. Von Stosch, M., Oliveira, R., Peres, J., & de Azevedo, S. F. (2014). Hybrid semi-parametric modeling in process systems engineering: Past, present and future. Computers & Chemical Engineering, 60, 86-101
5. Große, M., Viedt, I., Lange, H., and Urbas, L., (2024). Electrolysis stack modeling for dynamic system simulation of modular hydrogen plants, International Journal of Hydrogen Energy. (in review)
6. Bruckner, L., Oppelt, M., Urbas, L., & Barth, M. (2020). The current and future use of simulation in discrete and process industries. Siemens AG.
7. Lorenz, J., Klose, A., Lange, H., Kock, T., & Urbas, L. (2023, September). Process control principles for scalable electrolysis systems. In 2023 IEEE 28th International Conference on Emerging Technologies and Factory Automation (ETFA) (pp. 1-4). IEEE.
8. Viedt, I., Gopa, K. R., Mädler, J., & Urbas, L. (2023). Quality assessment of partial models for co-simulation of modular electrolysis plants. In Computer Aided Chemical Engineering (Vol. 52, pp. 1217-1222). Elsevier. https://doi.org/10.1016/B978-0-443-15274-0.50194-3
9. Viedt, I., Lorenz, R., & Urbas, L. (2024). Case study on quality assurance of third-party models for co-simulation using FMI. In Computer Aided Chemical Engineering (Vol. 53, pp. 3403-3408). Elsevier.
10. Glassey, J., & Von Stosch, M. (Eds.). (2018). Hybrid modeling in process industries. CRC Press.
11. Bae, J., Lee, H. J., Jeong, D. H., & Lee, J. M. (2020). Construction of a valid domain for a hybrid model and its application to dynamic optimization with controlled exploration. Industrial & Engineering Chemistry Research, 59(37), 16380-16395.
12. D. Bonvin, C. Georgakis, C. C. Pantelides, M. Barolo, M. A. Grover, D. Rodrigues, ... and D. Dochain, 2016, Linking models and experiments, Ind. Eng. Chem. Res, 55, 25, 6891-6903
13. Vincent, I., & Bessarabov, D. (2018). Low cost hydrogen production by anion exchange membrane electrolysis: A review. Renewable and Sustainable Energy Reviews, 81, 1690-1704.
14. Sinnott, R., & Towler, G. (2019). Chemical engineering design: SI Edition. Butterworth-Heinemann.
15. Sakas, G., Ibáñez-Rioja, A., Ruuskanen, V., Kosonen, A., Ahola, J., & Bergmann, O. (2022). Dynamic energy and mass balance model for an industrial alkaline water electrolyzer plant process. International Journal of Hydrogen Energy, 47(7), 4328-4345.
16. Nafchi, F. M., Afshari, E., & Baniasadi, E. (2024). Anion exchange membrane water electrolysis: Numerical modeling and electrochemical performance analysis. International Journal of Hydrogen Energy, 52, 306-321.
17. An, L., Zhao, T. S., Chai, Z. H., Tan, P., & Zeng, L. (2014). Mathematical modeling of an anion-exchange membrane water electrolyzer for hydrogen production. international journal of hydrogen energy, 39(35), 19869-19876.
18. Vidales, A. G., Millan, N. C., & Bock, C. (2023). Modeling of anion exchange membrane water electrolyzers: The influence of operating parameters. Chemical Engineering Research and Design, 194, 636-648.
19. National Renewable Energy Laboratory. Solar Power Data for Integration Studies 2024. https://www.nrel.gov/grid/solar-power-data.html (accessed November 14, 2024).
20. Zerrougui, I., Li, Z., & Hissel, D. (2025). Physics-Informed Neural Network for modeling and predicting temperature fluctuations in proton exchange membrane electrolysis. Energy and AI, 100474.
21. Lange, H., Klose, A., Lippmann, W., & Urbas, L. (2023). Technical evaluation of the flexibility of water electrolysis systems to increase energy flexibility: A review. International Journal of Hydrogen Energy, 48(42), 15771-15783.