

# Dynamic modeling of alkaline electrolyzers for diagnostic purposes



«Development of innovative models and techniques for the diagnostics and performance monitoring of alkaline electrolyzers»

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## 1 INTRODUCTION

Today, the interest in using hydrogen as an energy carrier, especially from renewables, is increasing. Models for simulating the operation of alkaline electrolyzers are available in the literature [1, 2], but they often overlook real-world issues like malfunctions and failures, which can compromise electrolyzer performance. Moreover, connecting them to fluctuating energy sources can lead to quick degradation and reduced lifespan.

### OBJECTIVES



## 2 METHODS

### FIRST PHASE - Modeling

Modeling of a 3MW alkaline electrolyzer using [2] as a reference, but with the integration of a temperature control to prevent overheating of the stack, and a liquid level control to prevent excessive filling or emptying of gas-liquid separators.

Implementation of the stack model using the MATLAB/Simulink software.

#### ELECTROCHEMICAL MODEL [2]

$$U_{cell} = U_{rev} + U_{ohm} + U_{act} + U_{con}^0$$

$$U_{rev} = U^0_{rev} + \left(\frac{R}{zF}\right) \ln\left(\frac{P - P_{v,KOH}}{P - P_{v,KOH}}\right) \left(\frac{P - P_{v,KOH}}{a_{H_2O,KOH}}\right)^{0.5}$$

$$U_{ohm} = (\alpha_1 + \alpha_2 T) i_{cell}$$

$$U_{act} = s \cdot \log\left(\beta_1 + \beta_2/T + \beta_3/T_2\right) i_{cell} + 1$$

#### PRODUCTION MODEL [3]

$$n_{H_2} = \eta_{Far} \left(\frac{i_{cell}}{zF}\right) U_{cell}$$

$$\eta_{Far} = \frac{(i_{cell})^2}{(f_1 + (i_{cell})^2) f_2}$$

$$f_1 = f_{11} + f_{12} T$$

$$f_2 = f_{21} + f_{22} T$$

#### THERMAL MODEL [1]

$$C_t \frac{dT}{dt} = \dot{Q}_{gen} - \dot{Q}_{loss} - \dot{Q}_{cool}$$

$$\dot{Q}_{gen} = n_{cell} i_{cell} (U_{cell} - U_{in})$$

$$\dot{Q}_{loss} = \frac{1}{R_t} (T - T_{amb})$$

$$\dot{Q}_{cool} = C_{cw} (T_{cw,out} - T_{cw,in}) = UA_{hx} \cdot LMTD$$

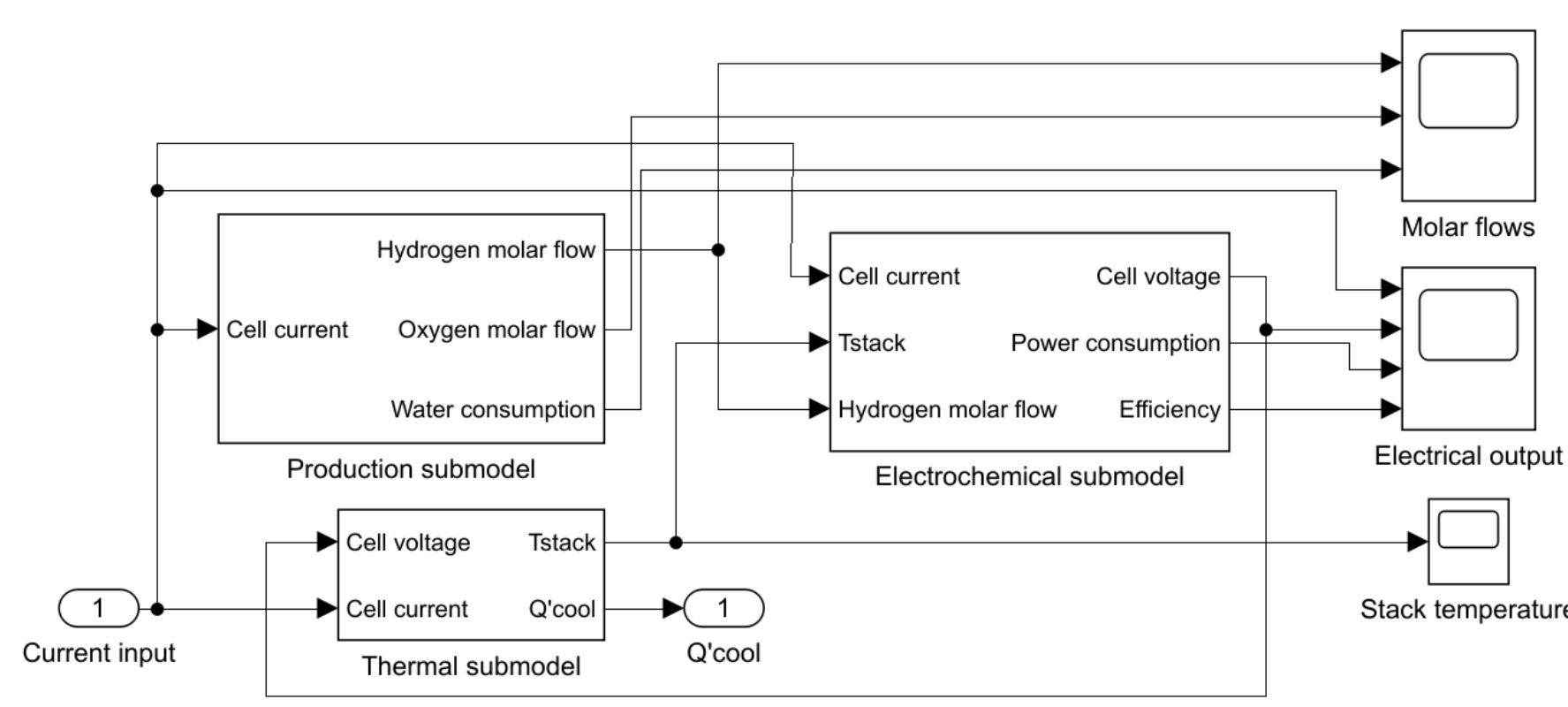


Fig.1 - Simulink stack model

#### Dynamic modeling of the electrolyzer in MATLAB/Simscape.

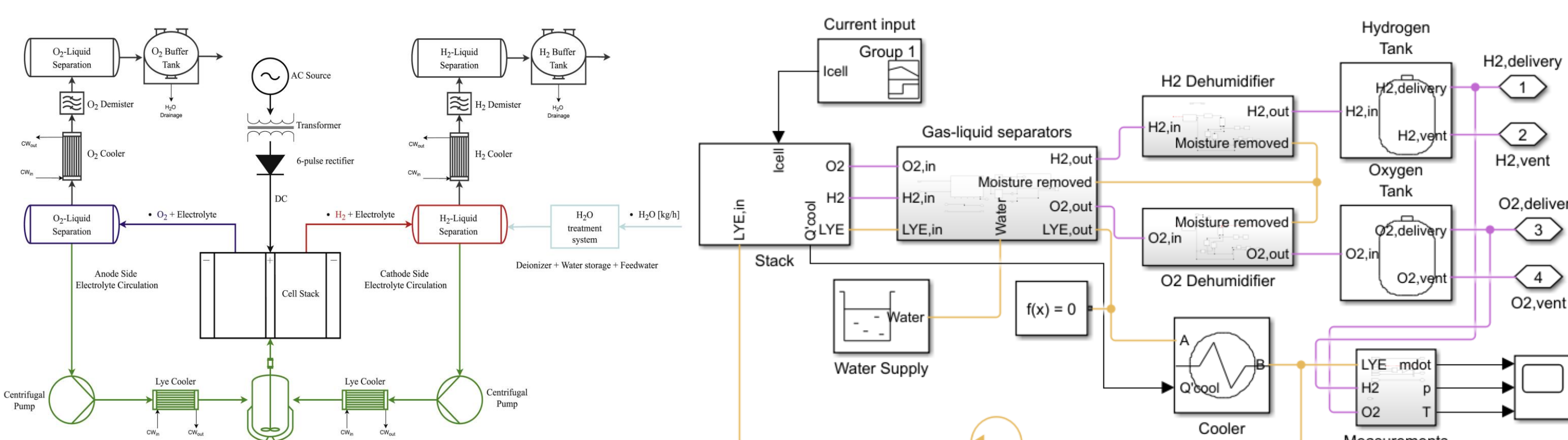


Fig.2 - Alkaline electrolyzer plant process diagram

Fig.3 - Simscape electrolyzer model

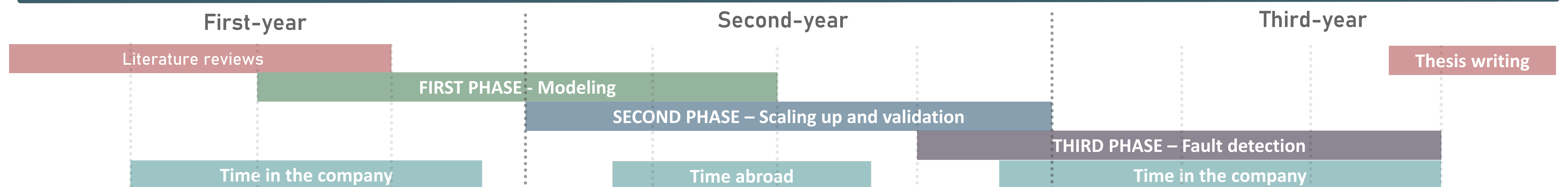
### SECOND PHASE - Scaling up and validation

Scaling up of the model using parameters from a real device.

Pressure [bar]	Hydrogen production nominal flowrate [Nm <sup>3</sup> /h]	Oxygen production nominal flowrate [Nm <sup>3</sup> /h]	Nominal power [kW]
8	10	5	60

Table 1 - McPhy Piel H-15 Hydrogen Generator operating parameters

## 5 TIMELINE



## 6 PUBLICATIONS and CONFERENCES

- V. Pignataro, A. Liponi, E. Bargiacchi, L. Ferrari. «Dynamic modeling of a power-to-gas system for green methane production from wind energy», in proceeding of the 36th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of energy systems, ECOS, 25-30 June 2023, Las Palmas de Gran Canaria, Spain (2023).
- V. Pignataro, A. Liponi, E. Bargiacchi, L. Ferrari. «Impact of management strategy on green methane production from wind energy», in proceeding of SUustainable PolyEnergy generation and HaRvesting Conference and Exhibition, SUPEHR23, 6-8 September 2023, Savona, Italy (2023).

## REFERENCES

- Ulleberg I. Modeling of advanced alkaline electrolyzers: a system simulation approach. Int J Hydrogen Energy, vol. 28, 2003, p. 21-3. [https://doi.org/10.1016/S0360-3199\(02\)00033-2](https://doi.org/10.1016/S0360-3199(02)00033-2).
- G. Sakas, A. Ibáñez-Rioja, V. Ruuskanen, A. Kosonen, J. Ahola, and O. Bergmann, "Dynamic energy and mass balance model for an industrial alkaline water electrolyzer plant process," Int J Hydrogen Energy, vol. 47, no. 7, pp. 4328-4345, Jan. 2022, doi: 10.1016/j.ijhydene.2021.11.126.
- M. Sánchez, E. Amores, L. Rodríguez, and C. Clemente-Jul, "Semi-empirical model and experimental validation for the performance evaluation of a 15 kW alkaline water electrolyzer," Int J Hydrogen Energy, vol. 43, no. 45, pp. 20332-20345, Nov. 2018, doi: 10.1016/j.ijhydene.2018.09.029.
- M. Maruf-ul-Karim and M. T. Iqbal, "Dynamic modeling and simulation of alkaline type electrolyzers," 2009 Canadian Conference on Electrical and Computer Engineering, St. John's, NL, Canada, 2009, pp. 711-715, doi: 10.1109/CCECE.2009.5090222.

Operational data collection from the stack and U-I curve fitting according to [1].

Validation of the model against measured data.

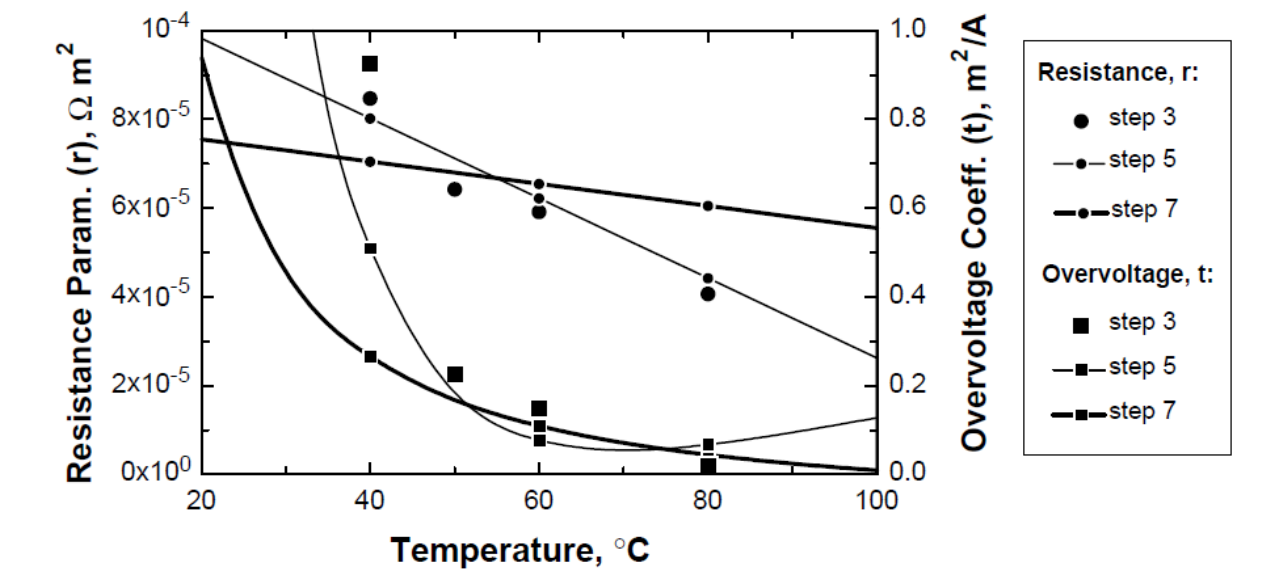
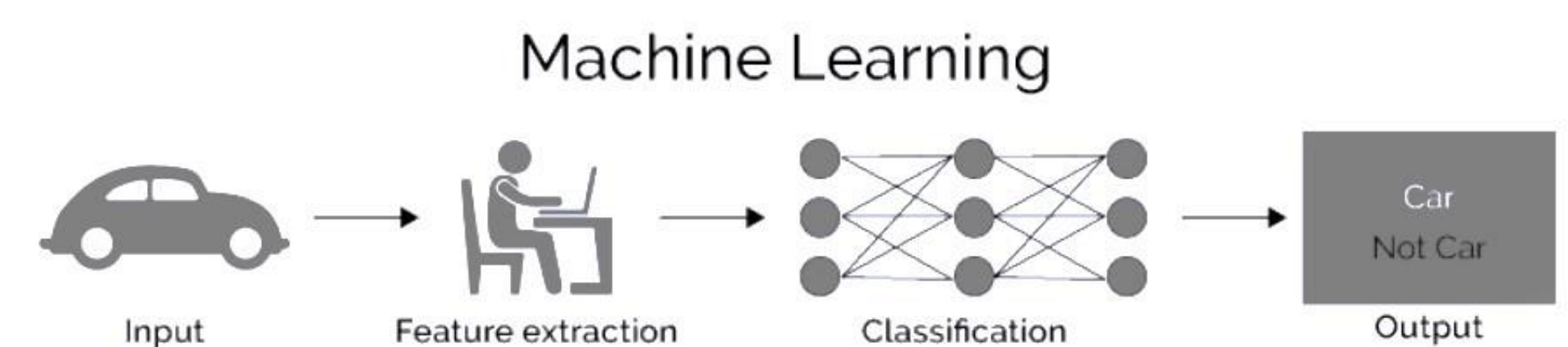


Fig.4 - Electrolyzer I-U curve fitting; illustration of a step-by-step procedure [1].

### THIRD PHASE - Fault detection

Machine learning model development using neural networks and regression algorithms.

Model training to identify patterns associated with faults.



Real-time monitoring of the electrolyzer performance.

## 3 PRELIMINARY and EXPECTED RESULTS

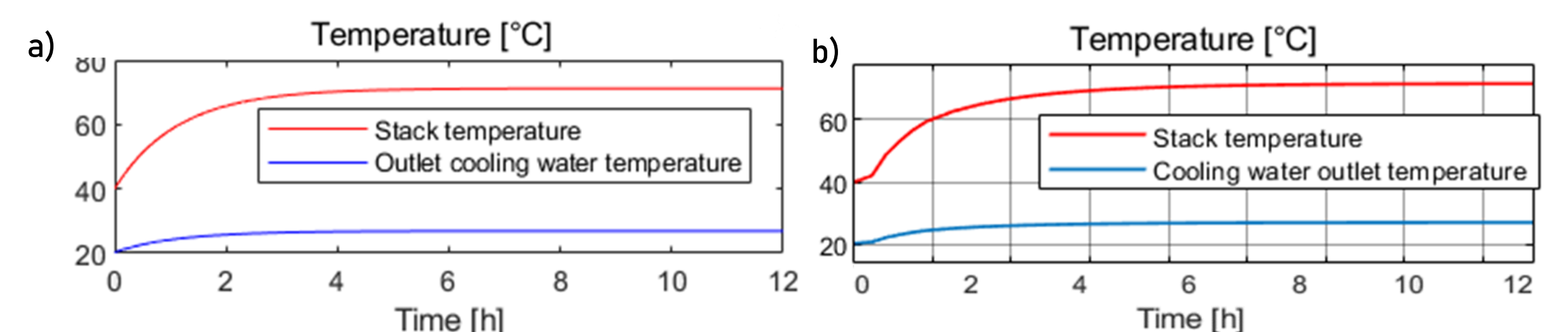


Fig.5 - Stack temperature and Outlet cooling water temperature of 3MW Matlab stack model (a) and 3MW Simulink stack model (b)

Results obtained by the simulation carried out with the Simulink model of the 3MW alkaline stack are very close to those obtained with the Matlab model, whose reference model [2] was validated.

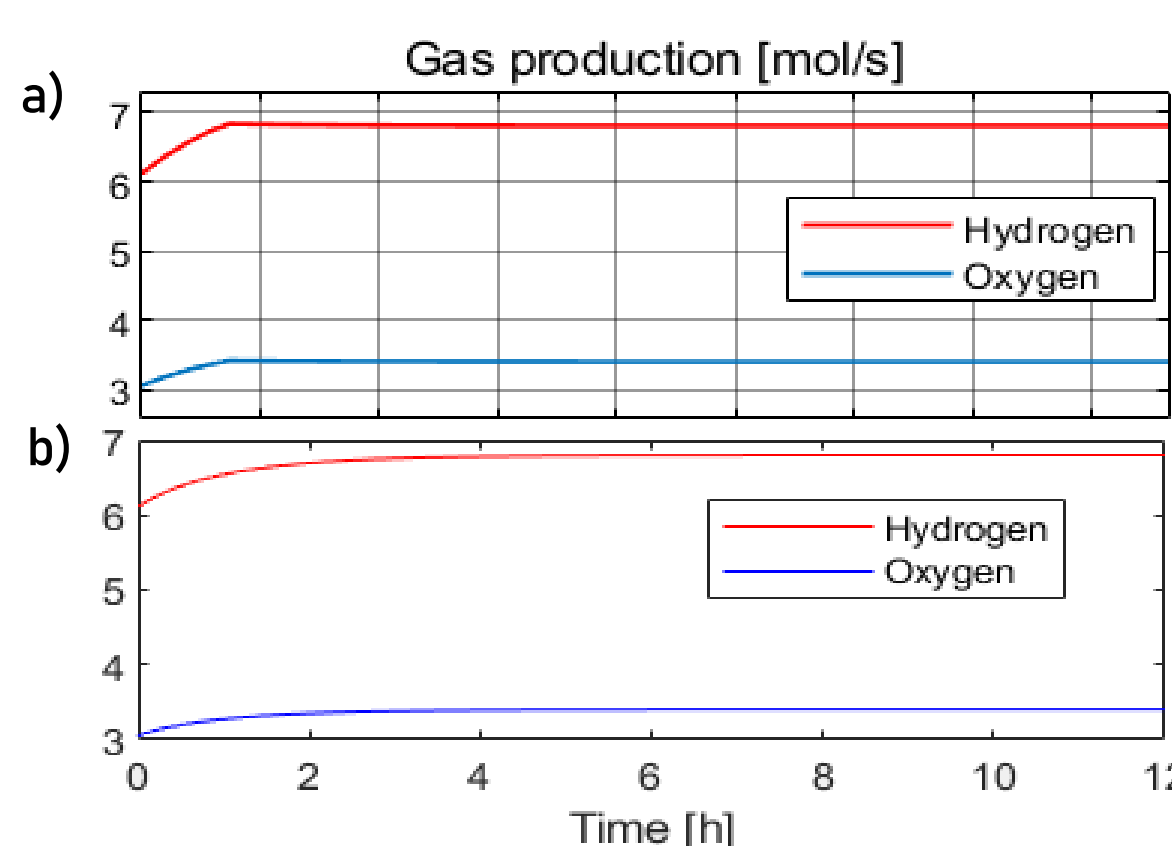


Fig.6 - Gas production flow rates of Matlab stack model (b) and Simulink stack model (a)

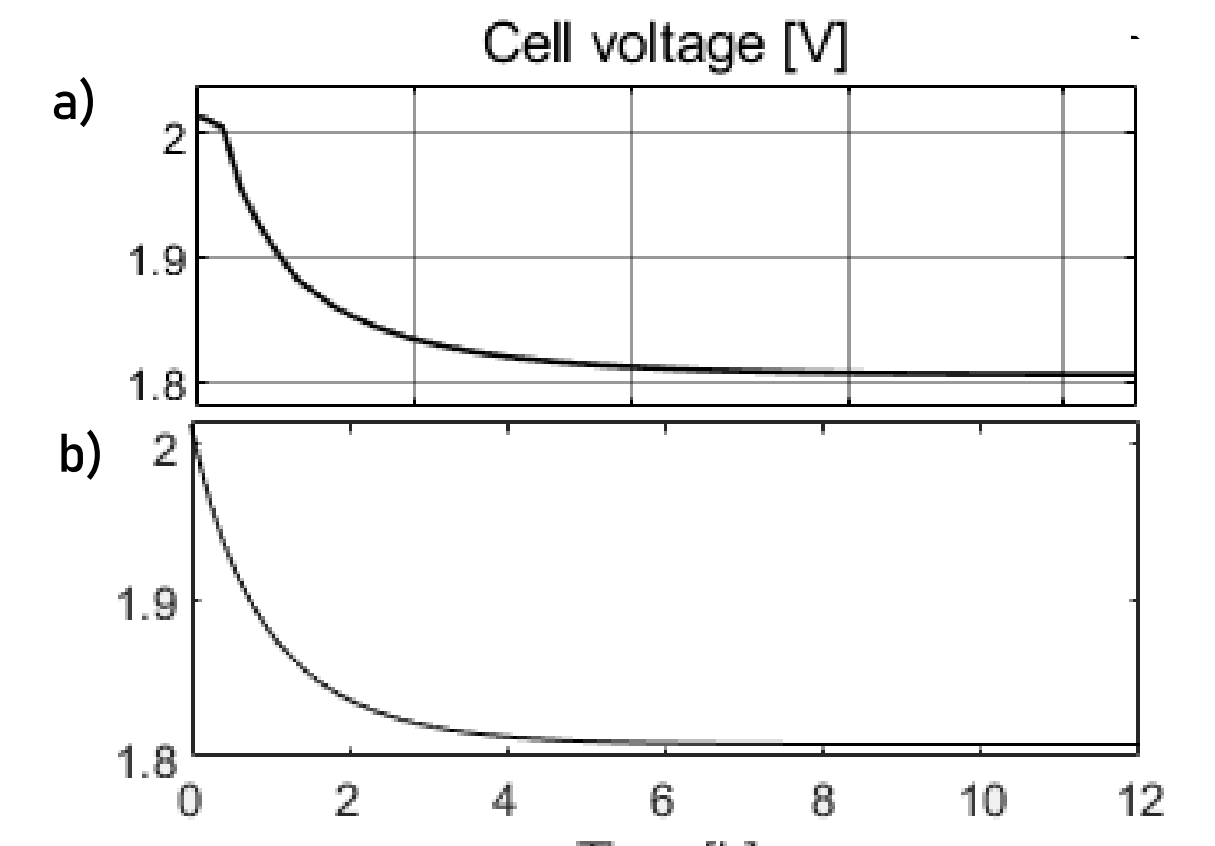


Fig.7 - Cell voltage of Matlab stack model (b) and Simulink stack model (a)

The developed model will be scaled and validated based on a real electrolyzer (McPhy Piel H-15 Hydrogen Generator) and will serve as the foundation for the development of a fault diagnostic tool.

The application of machine learning will offer a promising solution to enhance the prediction accuracy of the model.

## 4 CONCLUSIONS

- This research project started with the Matlab modeling of a 3MW alkaline electrolyzer, using the study by Sakas et al. [2] as a reference.
- The stack modeling will be implemented using MATLAB/Simulink and MATLAB/Simscape software.
- The model will be scaled up and validated using data from a real industrial device.
- The development of a fault detection and identification algorithm will offer a promising solution to enable timely corrective maintenance ensuring extended durability and reliability of the electrolyzer.