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Dynamic Operability Analysis of modular heterogeneous electrolyzer plants using system co-simulation

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ABSTRACT

In the upcoming decades, the scale-up of hydrogen production will play a crucial role for the integration of renewable energy into energy system. One scale-up strategy is the numbering-up of standardized electrolysis units in modular plant concepts. The use of modular plants can support the integration of different technologies into heterogeneous electrolyzer plants to leverage technology-specific advantages and counteract disadvantages. This work focuses on the analysis of technical operability of large-scale modular electrolyzer plants in heterogeneous plant layouts using co-simulation. Developed process models of low-temperature electrolysis components are combined in Simulink as shared environment. Strategies to control process parameters, like temperatures, pressures and flowrates in the subsystems and the overall plant, are developed and presented. An operability analysis is carried out to verify the functionality of the presented plant layout and control strategies. The dynamic progression of all parameters is presented for different operative states, like start-up, continuous operation, load change and hot-standby behavior. It is observed that the exemplary plant is operational, as all relevant process parameter can be held within the allowed operating range during all operative states. Some limitations, regarding the possible operating range of individual technologies, are introduced and solution approaches are conceptualized. Additionally, relevant metrics for efficiency, such as the specific energy consumption and flexibility are calculated to prove the feasibility and show the advantages of heterogeneous electrolyzer plant layouts, such as a heightened operational flexibility without mayor reductions in efficiency.

Keywords: Hydrogen, Modelling & Simulations, Process Control, Process Operations, MATLAB, Co-Simulation

INTRODUCTION & BACKGROUND

The rising demand for hydrogen and the necessary integration of fluctuating energy sources into chemical value chains remains a mayor challenge for the transition to renewable energy and a more sustainable chemical industry [1]. The numbering-up of standardized electrolysis units in a modular plant has been conceptualized as a reliable way to scale-up hydrogen production quickly [2]. Furthermore, the use of the modular plant concept allows for a more individualized and flexible scale-up by enabling the combination of modules from different providers. That way electrolysis plants can be designed to include different electrolysis technologies more easily to leverage technology-specific advantages and counteract disadvantages [2], [3]. The necessary components within such modular electrolysis plants of different technologies have been outlined in [4] and can be used as a reference for scale-up scenarios. An exemplary modular, electrolysis system is depicted in Figure 1. Before such plant layouts of pre-engineered and generic Process Equipment Assemblies (PEAs), can be connected and operated, the functionality and operability of such a heterogeneous plant layout of different technologies and varying PEA providers must be verified to ensure safe and efficient operation.

This paper aims to support this verification of heterogeneous modular electrolysis plants investigating the different steps of a dynamic operability analysis with a simple but exemplary use case as depicted in Figure 1.

The study aims to identify prerequisites and efforts as well as potential and limitations to prove safe and efficient operation of a such systems by assessing their ability to hold parameters within a Desired Output Set (DOS) [5]. In the context of modular plants and the integration of renewable energy sources in Power-to-X value chains, the dynamics of the plant must be taken into account to assess the plant operation during load or state changes [6]. This necessitates the calculation of specific metrics for dynamic operability evaluation of processes, as described in [7], on top of the steady-state operability. The necessary metrics shall be specified for the utilized use-case in the following chapter.

The depicted plant, consisting of individual modules from potentially varying suppliers, must therefore be simulated in an overall dynamic system simulation. As the internal knowledge of the modules is protected, the dynamic models are provided as black box models with their respective input-output behavior [8]. The black box models, potentially developed in different tools and with their individual solvers, are combined as Functional Mock-Up Units (FMUs) in a system co-simulation, as the Functional Mock-Up Interface (FMI) "enables an unprecedented level of integration of models (as black boxes) provided by different and even competing suppliers." [9]

METHODOLOGY

Definitions & Assumptions

Goal of the dynamic operability analysis is to provide proof, that a developed modular electrolysis system is operable. An operable process is defined as:

> "A process is operable if the available set of inputs is capable of satisfying the desired steady-state and dynamic performance requirements defined at the design stage, in the presence of the set of anticipated disturbances, without violating any process constraints." [7]

This necessitates the definition of varying aspects, that must be included in the operability analysis of modular electrolysis plants, such as the DOS, the dynamic Available Input Space (dAIS), the dynamic Desired Operating Space (dDOpS) and the Expected Disturbance Space (EDS) [5, 8]. The assumption of a modular plant design makes the variation of design input variables of the PEAs unsuitable, which is why the focus is on the operational variables of the PEAs. The ability to operate the combined heterogeneous modular electrolysis system out of predefined PEAs is to be evaluated.

A list of the included variables, their description and allowed ranges can be found in Tables 1-3 for the aspects of the operability analysis and their respective PEA. As each PEA encapsulates their individual behaviour and requirements, the presented method is applicable independently of the chosen plant layout. Due to limitations in the model capabilities, identified optima, simplifications or limited available data, the setpoints for some potential operating variables, such as the lye mass fraction or load change rates, are kept constant.

The dAIS entails the remaining setpoints, including the temperature, pressure and flow rate setpoints of the circulation and the production rate setpoint of the Stack-Unit. Additionally, the chosen lye mass fraction setpoint and load change rates over time are included in Table 1.

Table 1: Operating input variables in the dAIS and ranges taken from [2] or mapped to showcase from [10]

Operational input variable	Value/Range
Circulation: Outlet temperature setpoint [°C]	50-80
Circulation: Outlet flowrate setpoint [kg/s]	AEL: 30-90 PEMEL: 4.75-14
Circulation: Gas outlet pressure setpoint [bar]	3-16
Circulation: Lye mass fraction setpoint [m%]	30
Stack-Unit: Load setpoint [%]	20–100
Stack-Unit: Upramp load change rate [%/s]	AEL: 30 PEMEL: 50
Stack-Unit: Downramp load change rate [%/s]	AEL: 10 PEMEL: 40,6

The DOS includes the constraints, that apply for the PEAs, such as the allowed operating ranges for temperature, pressure, flowrate and component mass fractions in the entire system of PEAs. These constraints are extended by the dDOpS with the allowed change rates over time of the relevant parameters during nominal operation or in case of operational disturbances. The EDS includes the disturbances in the input variables that are assumed to enter the process, such as variations in the water inlet temperature or short outages of the cooling cycle.

Table 2: Output variables and dynamics in the DOS and dDOpS and allowed ranges assumed or adjusted from [2] and [10]

Output variable	Value/Range
Maximum allowed temperature in the Stack-Unit [°C]	AEL: 100 PEM: 90
Maximum temperature change rate in the Stack-Unit [K/min]	AEL: 1,5 PEMEL: 1
Maximum fluid velocity [m/s]	1
Maximum "H2 in O2" or "O2 in H2" values [mol%]	2
AEL: Maximum pressure difference between stack-sides [bar]	0.1

Table 3: Disturbances in the input variables and considered ranges

Input variable disturbances	Value/Range
Fresh water inlet / cooling water inlet / ambient temperature [°C]	15–30
Cooling cycle restart time [min]	5

These collected variables serve as the inputs and variations in the operability analysis of the heterogeneous modular electrolysis plant considered in this paper.

Calculated metrics

The calculated metrics within the operability analysis in this paper include the Achievable Output Set (AOS), the dynamic Achievable Operating Space (dAOpS), the Desired Input Space (DIS) and the dynamic operability.

The AOS is the "set of controlled variables that the system can achieve for the considered AIS and EDS." [5] In this case study, it includes the behaviour of the controlled variables in the system, such as temperature, pressure, flowrate and mass fractions, at steady state.

The extension of the AOS is the dAOpS as the "operating space representing the dynamic performance that can be achieved by the system for a given choice of the dAIS, DOS, and EDS." [7] That way the dynamic behaviour of the plant can be considered and violations of the maximum change rates or short-term deviations from the permitted working range can be identified.

The DIS is the "set of input values required for the system to reach all outputs in the DOS" [5], [7] and shall be identified by comparing the dAOpS and the DOS. The resulting edge cases, at which the dAOpS deviates from the DOS restrict the allowed operating range in the AIS and EDS, that are suited for compliance with the DOS.

In addition to the operability evaluations, the specific energy consumption and the "Lange-Große-Coefficient for hydrogen demand" (LGC_{H2}) of the system can be calculated from the simulated data for each operating point to determine optimal operating points within the allowed operating range. The specific energy consumption of the overall plant serves as a metric to determine an optimal operation scheme at least qualitatively. It is calculated as:

$$e_{spec}\left[\frac{kWh}{kg_{H_2}}\right] = \frac{P_{sys,cons}}{\dot{m}_{H_2,sys}} \quad (1)$$

With $P_{sys,cons}$ as the power consumption of the entire modular plant in *kW* and $\dot{m}_{H_2,stacks}$ as the combined produced hydrogen in all Stack-Unit PEAs in *kg/h*. For the scope of this paper, the efficiency evaluation is limited to the overall system efficiency at 100 % load.

The LGC_{H2} value shall serve as an initial measurement to assess the inertia and consequently the flexibility to output hydrogen for different system configurations or operating points. It can be calculated for each load step or for a production scenario according to:

$$LGC_{H2}\,[-] = \int_{t_{scenario,start}}^{t_{scenario,end}} \frac{abs(\dot{m}_{H_2,sys}(t) - \dot{m}_{H_2,sys,stat}(t))}{\dot{m}_{H_2,sys,stat}(t)}\,dt \quad (2)$$

With $\dot{m}_{H_2,sys}(t)$ as the current hydrogen production at time step t and $\dot{m}_{H_2,sys,stat}(t)$ as the stationary hydrogen production of the load setpoint at time step t, both in kg/h. The result is the part of the hydrogen production in %, that could not be met by the system and operating point under consideration for a production scenario.

Model capabilities & Implementation

The analysis is carried out as a co-simulation scenario of FMUs, that simulate the dynamic behavior of chosen PEAs identified in [4], namely the water supply, Stack-Unit and circulation PEAs, as depicted in Figure 2. Although the hydrogen purification PEA is neglected in the simulation the presented methodology is still applicable within the scope of this paper. The system simulation is set up in MATLAB Simulink as a co-simulation environment with the developed FMUs. In the context of protection of the PEAs internal knowledge a detailed description of the FMUs is not necessary for the presented method and beyond the scope of this paper. A basic description of the model, including capabilities, interfaces and setpoints shall suffice. A detailed model description and structure of the electrolyzer stack-units, the balance of plant components and control strategies shall be specified elsewhere [11].

The FMUs provide the dynamic input-output behaviour of the mass, components and energy in the individual PEAs to changes in their respective setpoints and inlets. The FMU interfaces follow the interface description in [12], providing ports for material streams, energy and information, such as setpoints for the controlled variables. Necessary system parameters of the individual technologies for the chosen scenario are taken from [13] for the AEL subsystem, are scaled from values in [14] for the PEMEL subsystem and are collected in Table 4.

Both subsystems are assumed to connect multiple Stack-Unit PEAs to one circulation PEA. Additionally, the circulation PEAs of each electrolyzer technology are both connected to the water supply PEA. For the scope of this paper, the only information exchange between the PEAs shall be the necessary supply of deionized water from the water supply PEA to the circulation PEA to hold the liquid level in the gas separation tanks constant. This necessary supply is used as the flowrate setpoint for the water supply PEAs internal flowrate control. The production load setpoint is used as input in the Stack-Unit PEA to control the hydrogen production rate. The operating variables temperature, pressure and flowrate in the Stack-Units and the rest of the system are controlled as setpoints in the circulation PEA. Restarting the cooling cycle is also controlled in the circulation PEA. Controlling these variables should suffice for the basic operation of the presented heterogeneous modular electrolyzer system.

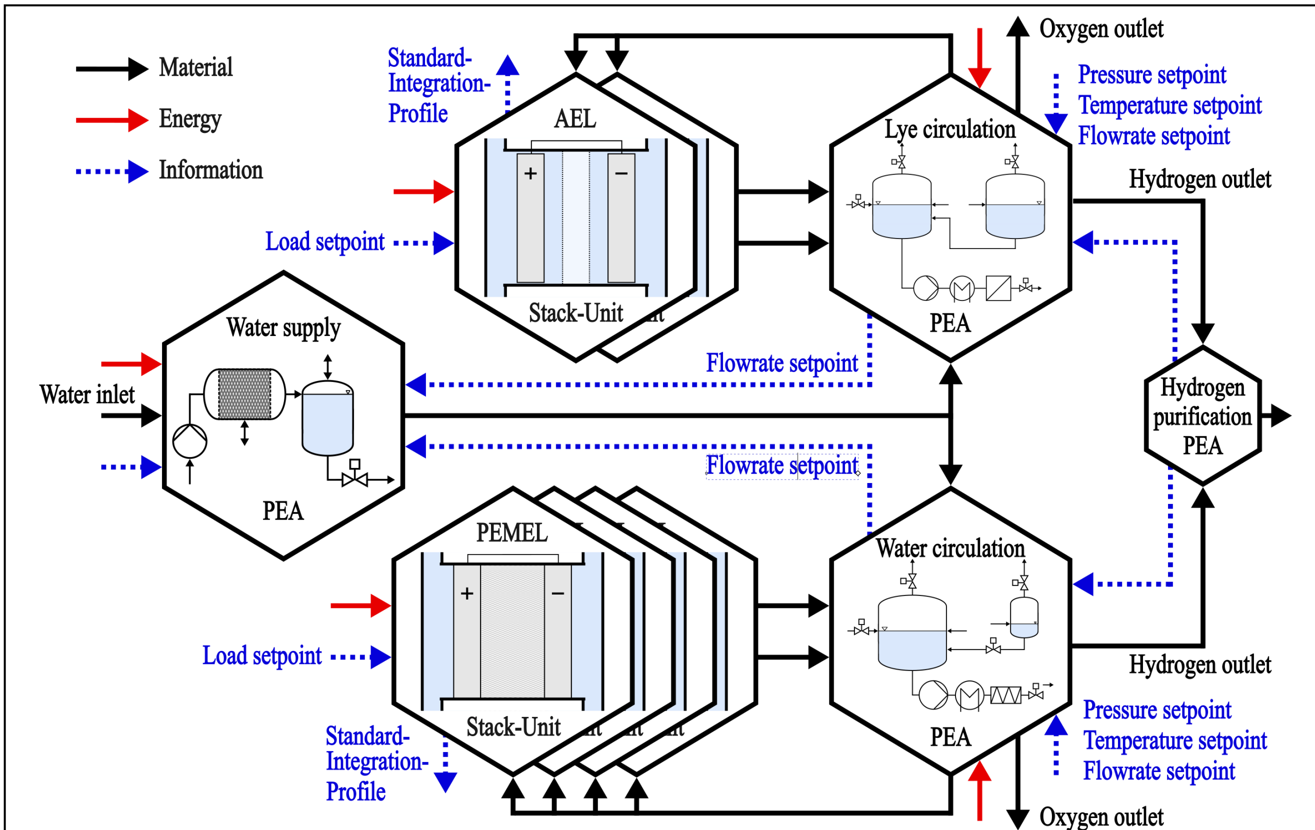

Figure 1: Exemplary modular, heterogeneous electrolyzer plant setup with considered material and information inlets and outlets in the dAIS and EDS

Table 4: Necessary system parameters of the individual subsystems taken or adjusted from [13] and [14]

System parameter	Value PEMEL	Value AEL
Number of Stack-Units per system [-]	4	2
Number of cells per Stack-Unit [-]	150	326
Active area of an electrolysis cell [m²]	87.5e-3	2.66
Nominal power of a Stack-Unit [MW]	0.25	3
Free volume of an electrolysis cell [m³]	8.75e-4	0.027
Separation tank volume [m³]	1.06	14.14
Maximum operating pressure [bar]	55	16

OPERABILITY ANALYSIS RESULTS

The operability analysis was successful as the modular, heterogeneous electrolysis system is operable in most of the operating states and ranges. However, at a few boundary conditions of the operating range and in the hot-standby state the DOS was exceeded, as shown for an exemplary inoperable operating point in Figure 2.

It can be seen, that at high temperatures, high pressures and low flowrates in the system, multiple criteria in the DOS are exceeded during nominal operation. The Stack-Unit outlet temperatures rise above the limit of 90 °C (upper left). Additionally, the H_2 in O_2 contamination in the AEL system exceeds the allowed threshold of 2 mol% at the 20 % Stack-Unit load setpoint (lower left). The temperature change rate during the cooling cycle shutdown rises above 1 K/min in the circulation however, in the Stack-Unit the temperature change rate stays below the threshold (upper right). The hot-standby state is not operable with the chosen PEAs and control strategies, as the difference pressure and the contaminations in the system rise above the set threshold in the dDOpS (lower left and right). Consequently, the current PEA selection and control strategies are not sufficient for the hot-standby state and complete operability is not given under the specified conditions. Further evaluations of specific energy consumption and LGC_{H2} shall therefore be done for the nominal operation state without consideration of the hot-standby state. The DIS for the nominal operation state can be seen in Figure 3 as the filled circles in the evaluation of specific energy consumption and LGC_{H2}. The unfilled circles represent the operating points, that are not operable in the nominal operation state with the chosen PEAs and control strategies.

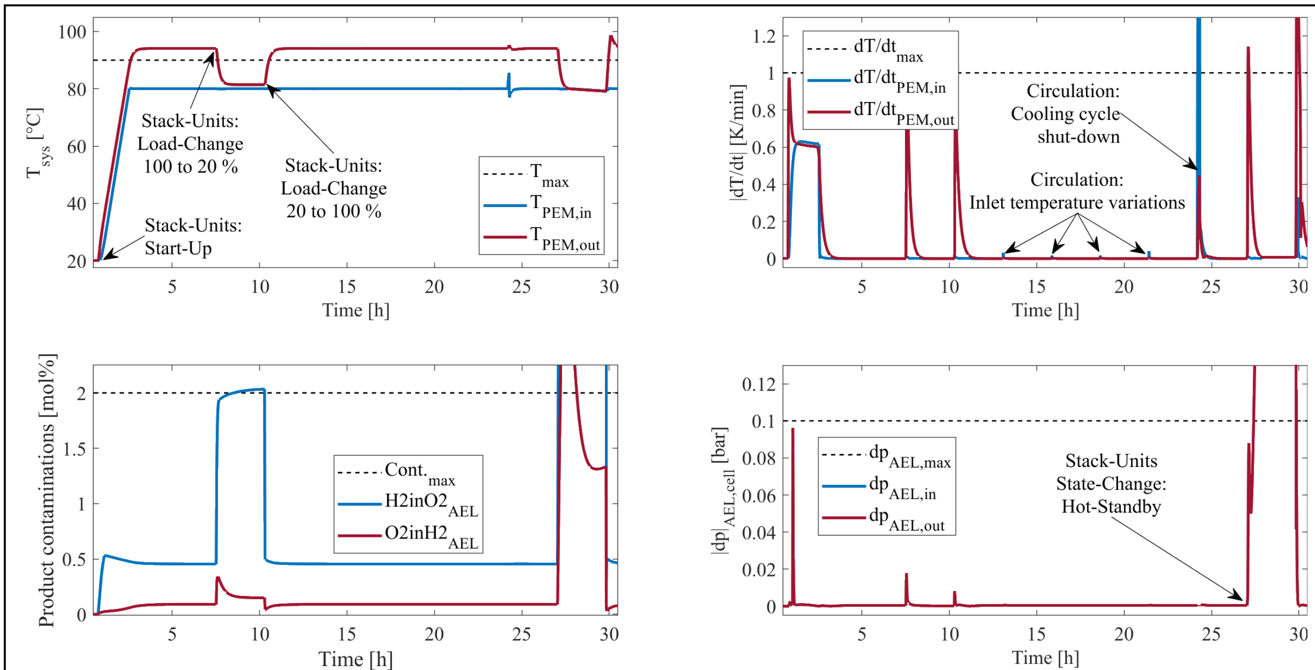

Figure 2: Examplary progression of relevant variables in the dAOpS with marked state changes for the dAIS setpoints: T_{Set} = 80 °C, p_{Set} = 16 bar, $f_{AEL,Set}$ = 30,6 kg/s & $f_{PEM,Set}$ = 4,76 kg/s

System efficiency and LHCH2

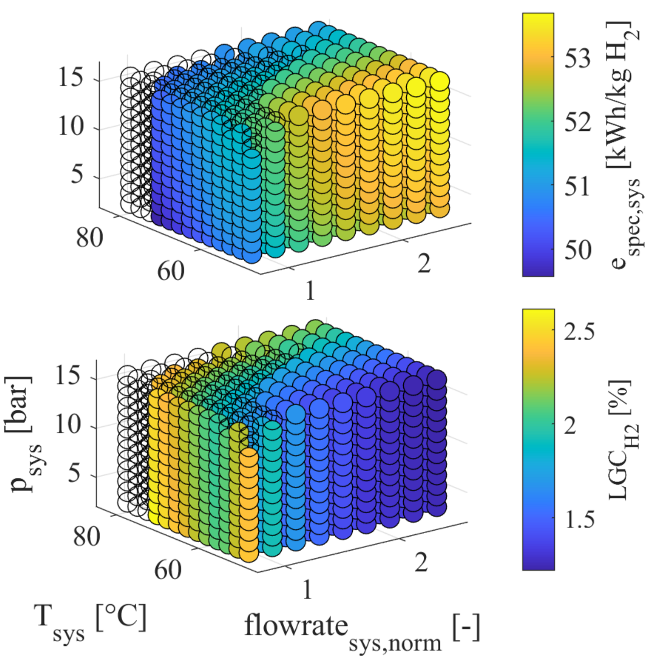

Figure 3: System efficiency and LGC_{H2} evaluation

The relevant system efficiency and LGC_{H2} are evaluated for all setpoints in the operable range of temperature, pressure and flowrate. Other system variables stay at their mean values in Tables 1-3. The results are depicted in Figure 3, with an optimal system efficiency of 49,57 kWh/kg H2, at the lowest pressure of 3 bar, the highest operable temperature of 72.5 °C and the lowest normalized flowrate of 0.85.

Limitations & Solution approaches

As the plant layout and control strategies have been simplified for the scope of this paper, some limitations to the significance and validity of the presented results must be made. The first aspect that must be considered for a more reliable operability analysis is the extension of the plant structure to include the purification and post-processing of produced hydrogen. The current results for system efficiency and LGC_{H2} are limited to the hydrogen generation and first separation stage leading to the assessment of high efficiency at lower pressures and high temperatures while neglecting potential losses due to necessary compression or drying of hydrogen in the post-processing. The inclusion of these steps in the operability analysis and system efficiency evaluation is necessary to provide a more meaningful understanding of electrolysis and their optimal operating conditions.

Secondly the hot-standby state can not be operated with the included control strategies due to a lack of inertization or strategies to deal with the gas crossover within the provided FMUs. Especially at high gas pressures, the difference in partial pressures between the hydrogen and oxygen side lead to a steady cross-over of gases in the hot-standby state. Without inerting or stopping the fluid circulation the contaminations and pressure differences between the gas sides rise.

CONCLUSION & OUTLOOK

In conclusion the operability of a modular, heterogeneous electrolysis system was verified with restrictions.

The possible operating ranges and variations in the operating regiment have been collected and introduced to a dynamic operability analysis. Extensive simulation studies using co-simulation of FMUs show the operability of the presented plant in most of the outlined operating range. Possible disturbances to the system inputs can be dealt with in the required time. Operating points for optimal system efficiency and flexibility of the plant have been identified, although the applicability to a more complex electrolysis system with downstream equipment is limited. For future work the presented solution approaches and additions to the system layout and control strategies with additional information exchange between PEAs, such as states and safety relevant variables, can provide a more comprehensive understanding of the operability and optimal performance of modular, heterogeneous electrolysis plants.

Digital supplementary material

The P2O Lab Learning Factory provides a Github-group repository which contains the individual model repositories of the developed simulation models. It is currently only available upon individual request at https://github.com/orgs/p2o-lab/teams/ap2_external/repositories. The repositories will be openly accessible starting from October 2025.

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