Experimental and simulative design of isothermal high temperature electrolyser controller for coupling with renewable energies

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Abstract

Electrolysis via solid oxide cells (SOC) shows unprecedent high electrical efficiencies, but transient SOC operating capabilities on a system level are still unclear and require the development of adequate control and operating strategies to minimize thermal gradients inside the reactors. In this study, we present an algorithm to maintain isothermal operating conditions in a SOC reactor. This algorithm has been created in an in-house simulation framework using a 24-stack model for different transient operating conditions, tuning the current demand of the reactor based on the fluctuating supply of fuel. Following, the simulation outcomes are validated in the experimental investigation, where the SOC reactor is operated dynamically, simulating a coupling with fluctuating energy sources. In the manuscript, the cardinal equations of the algorithm, and both simulative and experimental results will be shown in detail, eventually leading to a diminished temperature change of the SOC reactor of maximum 10 K. Ultimately, this approach leads to a faster response from SOC reactors in transient conditions, and can potentially drive a more widespread usage of the technology in combination with fluctuating energy sources. Analysis of the results will be presented to showcase a possible coupling between a SOC reactor and a renewable wind and/or PV source.

1 Introduction

Decarbonization is an urgent global challenge, with the transition to net-zero emissions requiring the efficient storage and conversion of renewable electricity into valuable feedstocks. Electrolysis is a key technology in this context, with various approaches currently available, including Proton Exchange Membrane Electrolysis (PEMEL), Alkaline Water Electrolysis (AEL), and Solid Oxide Electrolysis (SOE). Among these, solid oxide electrolysis cell (SOEC) reactors are particularly promising due to their high electrical efficiency, facilitated by high operating temperatures, which can be further increased by heat integration from external processes [1]. Solid oxide cells (SOCs) offer considerable versatility, capable of performing H2O electrolysis (1), CO2 electrolysis (2), or a combination of both, making them well-suited for integration with Power-to-X processes.

$$
2H_2O \to 2H_2 + O_2 \tag{1}
$$

$$
CO_2 + H_2O \rightarrow CO + H_2 + \frac{1}{2}O_2 \tag{2}
$$

Additionally, renewable energy sources (RES), such as offshore wind farms, can power SOC reactors to produce hydrogen or synthetic fuels, which can serve as energy carriers in downstream processes [2].

However, SOCs mainly are prone to mechanical damages since they mainly consist of brittle ceramic materials. For this reason, strong thermal gradients are generally avoided to mitigate thermal stresses in the stacks.

Furthermore, as discussed in [7], significant temperature gradients across the reactor can induce overvoltage in the cells, accelerating degradation processes. It is widely accepted that temperature gradients should be limited to the range of 5-8 K/cm to minimize these effects. In most current applications, isothermal operation is favoured which reduces thermal gradients in the reactor to a minimum. Hence, the dynamic operation of SOEC with RES causes the potential issue of evolving temporal and spatial temperature gradients and thermo-mechanical stresses. Nevertheless, dynamic operation can be facilitated by the development of adequate control and operating strategies on the reactor level. For instance, control strategies can focus on regulating the current supplied to the electrolyser, as this variable has the most direct impact on reactor temperature and different current densities may be required for different fuel gas compositions to keep the reactor isothermal. Existing research on SOC control strategies is limited, often focusing on single cells or stacks, as seen in studies [4-7]. These studies typically neglect the comprehensive system-level dynamics, including the Balanceof-Plant (BoP) components such as heaters, heat exchangers, and blowers, and fail to account for the interactions between different operating conditions of cells within large systems.

Further research [8-9] has explored control and operating strategies from a broader system perspective, yet these efforts lack validation in system-level setups and often do not utilize highly accurate transient models, which are essential for

capturing the time-dependent behaviours inherent in SOC processes [10-11].

In the present study, an automated control strategy to minimize thermal gradients during transient operation previously developed by simulation [12] is implemented experimentally on an SOC reactor with 24 stacks and a maximum of 120kWel to explore its transient operating capabilities.

.**2 Methodology**

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2.1 Simulative development of isothermal controller

This section details the development of the isothermal controller as outlined in [14]. The chapter is divided into two subsections: the first provides a concise overview of the simulation framework utilized for controller development, and the second describes the governing equations of the control system.

2.1.1 TEMPEST

Given the high operational costs and complexities associated with experimental testing, the controller was developed using an in-house simulation framework known as TEMPEST. This framework, built within the Madelia environment, is designed for simulating large-scale solid oxide reactors operating in both electrolysis and fuel cell modes. TEMPEST offers flexible simulation configurations, ranging from simplified 0D models to detailed representations of electrochemical phenomena occurring within a reactor, depending on the desired level of detail and the available computational resources. One of TEMPEST's primary applications is the development of operational strategies and control systems for solid oxide cell (SOC) reactors.

2.1.2 Governing equations of temperature controller

This section outlines the governing equations employed in the development of the temperature controller. The authors adopted a Multiple Input–Single Output (MISO) control approach, incorporating a mixed feedforward and PID control strategy. The MISO approach was selected to accommodate varying fuel compositions.

The mixed feedforward and PID control strategy allow the incorporation of precise equations and empirical data while retaining critical feedback from the reactor system. The feedforward component is based on Ohm's Law (3):

$$
U = I * R \tag{3}
$$

where *U* represents voltage (V), *I* is current (A), and *R* denotes the internal resistance (Ω) . In the SOC context, the highest contribution to the internal resistance is given by the Ohmic resistance and is usually expressed by the Area-Specific Resistance (*ASR*), expressed in Ω*cm².

The goal of the control strategy is to determine the required current adjustment *di/dt* to maintain isothermal operation (i.e., iso-voltage operation). Consequently, the authors modified Equation 3 as follows, as presented in [14]:

$$
i = i_{FF} + i_{PID} \tag{4}
$$

$$
i_{FF} = \frac{U_{id} - U_{tn}}{ASR} \tag{5}
$$

In Equations 4-5, all terms are area-specific to maintain dimensional consistency. The components of this equation are defined as follows:

- U_{id} is the Nernst potential, dependent on the average cell temperature and the mass fractions of the inlet fuels.
- U_{tn} is the isothermal voltage, defined as the ratio between the reaction enthalpy and the number of electrons to be converted, adjusted by the Faraday constant. It is also a function of temperature and fuel inlet composition.
- ASR is the total ohmic area-specific resistance of the cell, derived from an exponential correlation established through in-house experiments, as detailed in [16].
- i represents the current density $(A/cm²)$, a standard parameter in SOEC studies indicating the current passing through each square centimetre of the cell module.

Additionally, a feedback loop incorporating a PID controller is integrated to correct any deviations in the feedforward calculation. The PID controller uses the maximum cell temperature as the setpoint and the current delta as the process variable, ensuring precise temperature control across the reactor.

2.2 Implementation on large-SOEC test rig

This section outlines the implementation of the control algorithm on a large SOC test rig. The chapter begins with a brief overview of the test rig, emphasizing its unique features, followed by a general description of the control system algorithm. Finally, the specifics of the final implementation are presented.

2.2.1 GALACTICA

As previously discussed, one of the primary challenges in the widespread adoption of SOC technology is the difficulty in scaling up reactor designs. This issue is exacerbated by the scarcity of large-scale test reactors available at research institutions, which hinders the proper validation of operational strategies and control systems.

To address this gap, the DLR-EHT has developed the test rig GALACTICA, which offers a unique platform for

investigating large SOC reactors from various manufacturers. GALACTICA supports operation both as a Solid Oxide Fuel Cell (SOFC) for power generation, with a capacity of up to 40 kwel, and as an SOEC for hydrogen and syngas production, with an electrical power input of up to 120 kWel. Additionally, GALACTICA enables reversible SOC (rSOC) operation, facilitated by its bi-directional power electronics, allowing seamless transition between SOFC and SOEC modes.

2.2.2 GALACTICA Control System

The GALACTICA control system is designed to facilitate efficient communication of input and output signals between the test rig's supporting elements, the reactor itself, and the main operating PC.

At the core of the control system is a National Instruments CompactRIO (NI-cRIO) module. This module plays a critical role in the operation by acquiring real-time data from various system components and transmitting this information to the main PC (referred to as the HOST-PC), as illustrated in Figure 1. The NI-cRIO also facilitates the reverse process, where control commands issued from the HOST-PC are relayed to the appropriate hardware components as setpoints.

The communication between the control system and the hardware components is handled through multiple protocols, depending on the specific hardware in use. These protocols include analog and digital signals, as well as RS232, EtherCAT, and MODBUS-TCP.

Figure 1: Overview of the control communication in GALACTICA

This setup ensures that the GALACTICA test rig can precisely control and monitor large-scale SOC operations, providing a robust platform for validating control strategies and advancing SOEC technology.

2.2.3 Temperature controller implementation

In this subsection, a description of the controller logic in the test rig is given. A block diagram of the algorithm is also shown in Figure 2.

Figure 2: Temperature controller algorithm

The first step in the control algorithm is to determine whether the controller is active, which is managed by a Boolean variable within GALACTICA's test rig software. If this variable is set to 0, the controller is bypassed, and the test rig operates in manual mode. If the variable is set to 1, the controller becomes active and generates a global variable, enabling the transfer of controlled signals to the test rig.

Once activated, the controller retrieves real-time mass flow data for all fuel components from the BoP components. Using this data, the controller calculates the mass fractions of steam (y_{H_2O}) and carbon dioxide (y_{CO_2}) using the equations (6) and (7):

$$
y_{H_2O} = \frac{m_{H_2O}}{\Sigma m_i} \tag{6}
$$

$$
y_{CO_2} = \frac{m_{CO_2}}{\Sigma m_i} \tag{7}
$$

The test rig also records temperature readings from thermocouples located within the stack. The controller uses the average of these readings to calculate key parameters such as the ASR, the ideal voltage, and the thermoneutral voltage, as described in Equation 2.

Simultaneously, the average temperature is monitored by the controller and fed into a PID controller. The temperature input is limited to a slew rate of 5 K/min to prevent excessive temperature gradients that could adversely affect the

controller's performance. The PID controller is tuned using the Ziegler-Nichols method [17], with the following tuning parameters:

The PID output is constrained to operate within a predefined range, with the upper limit determined by the thermoneutral voltage and the lower limit set at 45A, in accordance with the manufacturer's specifications. This bounded output is then combined with the feedforward component, completing the calculation described in Equation 2.

To ensure safe operation, the sum of the PID output and feedforward control is also restricted by a slew rate of 10 A/min. Finally, a replicator is employed to distribute the controlled current value across multiple parallel electrical circuits, ensuring consistent and stable operation of the system.

3 Results

In this chapter, two sets of results are presented in detail. The first scenario simulates the start-up phase of a SOC reactor when connected to an external energy source. This scenario examines the reactor's behavior as it transitions from an idle state to active operation. The second scenario focuses on a transient operation of the SOC reactor, demonstrating its capability to operate at various points of operation in response to changing external conditions. These simulations provide insights into the reactor's flexibility and responsiveness under different operational scenarios.

3.1 Scenario 1

The first set of results replicates the transition from an idle condition (HTSBY) to isothermal operation at 70% nominal load. As the thermal gradient limits are stricter during Co-Electrolysis due to potential cell damage, the standard procedure involves the transition from HTSBY to isothermal operation in H₂O-electrolysis mode and a subsequent switch to Co-electrolysis as it is shown n Figure 3b. With such an operating strategy, evolution of the highest thermal gradients have been shown to take place during steam electrolysis minimizing the risk of SOC reactor damage [12].

The details of the operating points can be found in Table 2. To be noted how the remaining amount of volume fraction of the gases is made by hydrogen flow.

Figure 3a depicts the controlled current during this transition phase. Around the 280-minute mark, a noticeable oscillation occurs due to the activation of the controller by setting the Boolean variable *isActive* to TRUE (as shown in Figure 2).

Figure 3: Results of scenario 1

Figure 4: Results of scenario 2

This oscillation is caused by the PID controller's need to quickly adjust to the actual current value at that moment.

Once the PID controller stabilizes, the current steadily increases, ultimately reaching the target of 70% COelectrolysis load. This rise in current is necessary to compensate for the potential temperature drop associated with the change in gas composition which is caused by the onset of the endothermic reverse water gas shift reaction during co-electrolysis.

In Figure 3c, the temperature profile for all the stacks can be seen. At the moment of the switch in composition (t~=280min) it can be noted an increase in temperature due to the increasing current: this can be attributed to the controller operation, as it was tuned with higher current profiles in mind. Hence, the current profile rises faster than what is needed for partial loads. Nevertheless, the behavior at a lower percentage of load is still considered acceptable and inside the limits of safe operation for the reactor. After approximately 80 minutes from the switch $(t=360\text{min})$, some of the reactor stacks began to exhibit a temperature increase due to unknown reasons. The controller responded promptly by reducing the current, thereby re-establishing isothermal conditions and effectively maintaining the reactor's thermal stability even in the case of an unforeseen event.

3.2 Scenario 2

The second scenario explores transient operation at various load points. Initially, the reactor transitions from the idle condition to H₂O-electrolysis, as described earlier. Following this, the reactor operates at three distinct points in coelectrolysis (Figure 4a), each maintaining isothermal conditions. This scenario provides a sped-up simulation of

the reactor's response to different downstream processes, resulting in varying operating points.

Figure 4b illustrates how the fuel composition is adjusted to accommodate changes in available power, simulating a transient response to fluctuations in input current. As power levels fluctuate, the controller adapts the current value to sustain isothermal conditions. This adaptability ensures stable operation both during transient changes and in steady-state conditions, as demonstrated in Figure 4c and 4d.

In this case, the temperature profile does not show the oscillation seen in figure 3c: this is further proof of the controller operation being accurate at full load for the reactor.

The resulting values of this scenario are illustrated in the following table:

Table 3: Operating points of Scenario 2

4 Conclusion

In this paper, the authors implemented and tested a previously developed temperature controller for a SOC reactor on a largescale system test rig to explore SOC thermal behaviour during transient operation. The primary aim of this operation is to mitigate thermal gradients to enable integration of SOC reactors with renewable energy sources, ensuring a stable and reliable supply of hydrogen $(H₂)$ and carbon monoxide (CO) for downstream processes. The investigation yielded

promising results, demonstrating the feasibility of maintaining stable operation under varying conditions. These findings represent a significant step forward in the upscaling of SOC reactors and their integration with renewable energy systems. Further development will go in the direction of improving the behaviour of the mentioned controller at partial loads and in implementing real-life energy profiles to properly match existing conditions.

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