

Techno-economic assessment of SOEC

Identifying potentials for grid integration

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August, 2019

Acknowledgement

This is an internal report prepared as part of the project *Coordinated Operation of Integrated Energy Systems*, hereafter abbreviated as **(CORE)**, supported by the Energy Technology Development and Demonstration Programme (originally, Det Energiteknologiske Udviklings- og Demonstrationsprogram (EUDP)) through the grant 64017-0005. The authors would like to extend their gratitude to all the project partners from DTU Electro, Aalborg University, Vestas Wind Energy Systems A/S, and Danfoss A/S for many important sessions of fruitful discussions and feedback. Additionally, the authors are very grateful for the contributions provided by many individuals, including Søren Højgaard Jensen, Christopher Graves, Allan Schrøder Pedersen, and Mogens Bjerg Mogensen for their valuable input in the subject matter.

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31 May 2019

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Abstract

Power to Gas (P2G) technology is envisioned to play a dominant role in future hydrogen production from renewable electricity sources, thereby providing an efficient route for replacing fossil fuels. While there is a general agreement on the importance of water electrolysis for hydrogen applications in future, it is worth noting that the views on commercial deployment of this energy storage vary widely among stakeholders and manufacturers. The primary challenges of this technology, especially for the solid oxide electrolysis cells (SOECs), include high capital cost of the electrolyser unit and auxiliary systems, improving energy efficiency, prolonging stack lifetime by reducing the effects of thermal stress.

The following report takes an in-depth look at the realistic scope of SOEC commercialization for mid-term (2030-2040) Danish power system. Given the wide range of topics covered by the broad aim placed in this work, discussions are focused to three selected topics. These are efficiency, ramping ability, and economic attractiveness of SOECs.

There are several factors that can influence stack efficiency. It can be beneficial to apply an operating strategy to minimize waste heat generation. Additionally, presence of facilities nearby providing steam directly to the SOEC inlet can largely enhance system performance. In order to counteract the excess heat generation within the stack, a new operating strategy is proposed here that allows for continuous system modulations while balancing internal heat of the stack. If the cell temperature is maintained at the operating temperature, fast regulation abilities can be achieved with power shifting from 0% to 100% within a few seconds. This ramping flexibility opens up new opportunities for energy market players, especially those willing to offer secondary and tertiary reserves in the intra-day electricity market.

Abbreviations

AC:	Alternating Current
ASR:	Area Specific Resistance
BoP:	Balance of Plant
CAPEX:	Capital Expenditure
CFD:	Computational Fluid Dynamics
CORE:	Coordinated Operation of Integrated Energy Systems
DC:	Direct Current
DOE:	Department of Energy
DTU:	Danmarks Tekniske Universitet
EC:	Electrolysis Cell
EUDP:	Energiteknologiske Udviklings- og Demonstrationsprogram
FC:	Fuel Cell
HHV:	Higher Heating Value
HTSE:	High Temperature Steam Electrolysis
INL:	Idaho National Laboratory
LHV:	Lower Heating Value
NIST:	National Institute of Standards and Technology
O&M:	Operation and Maintenance
OPEX:	Operating Expense
P2G:	Power to Gas
PEM:	Proton Exchange Membrane
R&D:	Research and Development
SOC:	Solid Oxide Cell
SOEC:	Solid Oxide Electrolysis Cell
SOFC:	Solid Oxide Fuel Cell
US:	United States
WP:	Work Package

1 Introduction

Hydrogen gas has been identified as a universal energy carrier since it is environment friendly, and contains high gravimetric energy density. Due to these features, hydrogen production via electrolysis of water is now considered a key technology towards sustainable power system. Among all known electrolysis technologies, high temperature steam electrolysis in Solid Oxide Electrolysis Cell (SOEC) is gaining substantial interest due to improved reaction kinetics, high efficiency, inexpensive cell materials, and possibility to operate in reverse mode as a fuel cell. However, this technology is still in the research and development (R&D) stage and the first commercial systems has barely been deployed. In order to facilitate commercialization and market acceptance, SOEC research must circumvent major challenges, like thermal stress causing shortened stack lifetime, high cost of stack modules, and complex fabrication issues. Also, the state-of-the-art SOECs suffer from significant degradation (increase in cell resistance) at high current densities, which is otherwise desired to ensure increased production of hydrogen and thereby improving the overall economy.

This report is prepared as a part of the project *Coordinated Operation of Integrated Energy Systems*, shortened to **CORE**, to answer some of these challenges from a system perspective. This project is intended to develop a holistic design and operation of a 100% renewable based energy systems with power-to-gas (P2G) technologies ensuring security of the whole system. As a result, designing a cost-optimal operation of a P2G plant builds the key to the WP2 of this project. While this P2G model development is exclusively a part of the WP2, other work packages intend to use this to answer important research questions on topics such as flexibility and ramping requirements in Danish power system (WP3), designing a market framework and business model (WP4), finding optimal dispatch strategies (WP5), and finally, real time demonstration (WP6). Due to the diversity of these packages, three important topics regarding SOEC behavior have been selected to discuss in this report, in order to provide anyone with specific values and understanding related to SOEC system integration. These are the efficiency, ramping requirements to assess regulation abilities, and the economic analysis of the SOEC system.

This report is organized as follows: Section 2 outlines the current status of Solid Oxide Cells (SOCs) with a brief overview of ongoing research from literature review, in Section 3 the theoretical background of SOCs operation is given in a very concise manner, Section 4 gives an overview of the SOEC model. In the following three sections, Section 5, 6, 7 discussions are made on efficiency calculations, ramping requirements in system regulations, and some economic aspects. As mentioned above, these topics are presented here in the context of project's overall aim and interest. The report is ended with a summary and outlook on possible future direction.

2 Brief status of SOC research

Majority of the research work carried out so far in the field of fuel cell research are primarily covered by experimental studies. While these experiments provide adequate information on overall cell performance, they can be very challenging in terms of monitoring and maintaining in-situ conditions. Additionally, these experiments can be quite time consuming and expensive. Instead, it can be beneficial to use numerical simulation tools to get a deeper understanding of hydrodynamic and electrochemical interactions which is fundamental in further improvement of these electrolysis cells¹. Hence, it is important to develop modeling tools to acquire these insights, but only a little work has been done so far in this direction.

Among the limited number of modeling studies in this field, most include simulation of thermal, chemical, and electrochemical behavior of single cells or multi-cell stacks. While some of these studies have focused on energy and exergy analysis on the system level^{2,3,4,5,6}, others are attributed in understanding hydrodynamic and electrochemical issues within the stack by looking into electrode micro-structures and design elements^{7,8,9}. With the gradual advancement in computational resources, multi-dimensional (1-D, 2-D and 3-D) computational fluid dynamic (CFD) models have been developed^{10,11,12} which provide excellent insight of fluid and heat distribution within the stack.

In an effort to improve system performance, significant attention has been given to material selection and cell configurations to ensure improved operational performance^{13,9,14} and to minimize thermal degradation and prolong system's lifetime^{4,15,16,17}. Performance analysis in SOC research is often evaluated against various parameters such as flow rate, mixing ratio, design geometry (such as, distance between the electrodes, thickness of electrolyte, gas flow direction etc.)^{18,19}.

In order to understand economic attractiveness of SOCs with respect to other competitive technologies, it is important to harness some effort in economic analysis. Since SOC is still not a mature technology and currently exist only on lab scale, studies covering details on their economic viability is extremely rare. Jan Thijssen from the US Department of Energy (DOE) did an extensive study on the effects of scale-up and production volume on SOC manufacturing cost²⁰. In 2017, a group of researchers from Imperial College London did an elicitation study for future SOC cost projections, by consulting different academic and industrial experts²¹. The impact of heat management and to identify the key parameters to achieve low production cost have long been the focal point of SOC cost analysis due to unforeseen business opportunities and market integration^{22,23,24,6,25}.

3 Theoretical background

In an attempt to establish an efficiency expression (Eq. 10 in Sec. 5), it is important to first understand the theoretical background of water electrolysis. In the following sections, the basic background of water electrolysis is discussed focusing on the thermal management of stack that directly influences the efficiency. More details on thermodynamic and electrochemical characteristics are presented in Appendix. A and B, respectively.

3.1 Fundamentals of water electrolysis

Electrolysis of water is a well-known concept that has been used across various industrial sectors (such as, food industry, power plants, metallurgy etc.) for over a century now. It has now been identified as a potential source of high-purity hydrogen and a green energy storage medium for power grids with large shares of fluctuating renewable energy sources. The basic reaction scheme of water electrolysis can be written as:



The reversible sign of Eq.1 signifies a potential for reversible operation, with the forward reaction indicating the electrolysis mode (EC) whereas the backward reaction showing the fuel cell (FC) mode. While the forward reaction is endothermic (requires both electric and heat energy input), the fuel cell mode is exothermic, thereby producing electricity and heat energy during the processⁱ. This unique quality opens up an opportunity for their usage as energy storage systems by absorbing the surplus electricity from the grid by running in the electrolysis mode and makes it possible to produce electricity in fuel cell mode during the hours of electricity deficit in the grid. With increasing shares of fluctuating renewable energy sources in the grid, such storage systems can withhold the potential for a viable business opportunity. For this work, as far as the project is concerned, the focus is mainly kept on the EC mode for usage of H_2 in electro-fuel production, although the developed model (discussed in details in Sec.4) has the potential to run in either direction, as required by the user. For the rest of this section, all discussions will be directed towards the electrolysis mode, unless stated otherwise.

Although electrolysis of water requires both electrical energy and heat for the reaction, the relative share between these two forms of energy is strongly dependent on operating temperature. Fig.1 shows that electrical or the useful form of energy (the Gibbs free energy) requirement strongly decreases with increasing temperature, while the overall enthalpy remains almost unaffected by changing temperature. This indicates that electrolysis of a given amount of reactant at elevated temperature can be extremely beneficial as expensive electrical energy can be compensated by low-cost heat. In addition, reaction kinetics is also significantly improved with increasing temperature, thereby leading to a favor for the High Temperature Steam Electrolysis (HTSE), which is often aided by the SOC technology. While other competing technologies such as Alkaline and PEM electrolysis cell operate below 100°C on liquid water, SOC operates on high temperature steam, around 650 - 1000°C. Although this elevated temperature has some advantages, it also induces additional challenges such as development

ⁱStrictly speaking, electrolysis mode need not always be endothermic. Depending on the operating voltage, it can be either endothermic or exothermic or maybe even thermoneutral. This is further discussed in 3.2

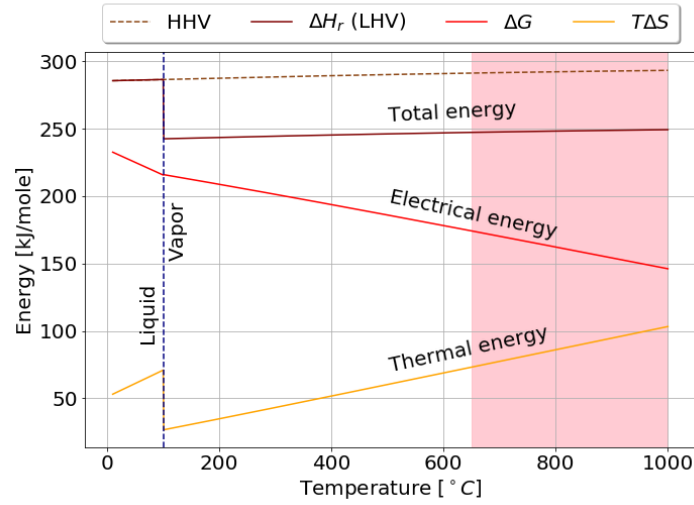


Figure 1: Changes in enthalpy (ΔH) and shares of electrical (given as ΔG) and thermal energy (given as $T\Delta S$) needs with increasing temperature.

of thermo-mechanical stress within the cell, possibility of stack degradation due to this stress, and long start-up times when the plant is activated from cold conditions. In order to overcome these challenges, it is important to understand thermo-mechanical and electro-chemical behavior of SOCs under various operating conditions via detailed model analysis. Further details on thermodynamic and IV characteristics of SOC are briefly presented in Appendix A and Appendix B, respectively.

3.2 Heat management in electrolysis mode

The thermal behavior of the SOC is influenced by the operating condition, in relation to the so called thermoneutral voltage, V_{tn} . Several studies have analyzed how thermoneutral voltage is affected by stack operating parameters, such as temperature, pressure, inlet gas composition etc.^{26,27}. The concept of thermoneutral voltage is popularly applied to both steam and co-electrolysis in the context of thermal management. It is a useful parameter to quantify the heating or cooling requirements in the stack.

In the context of steam electrolysis, the electrochemical reaction is endothermic, thereby requiring reaction heat to be provided in addition to electrical energy. However, there is simultaneously generation of heat within the cell due to resistance against moving currents. Thermoneutral voltage is the term used for the potential where the heat consumed by the electrolysis reaction and the Ohmic heat created in the stack are equal. It is typically defined as the change in enthalpy (i.e., heat of reaction, ΔH) associated with electrochemical reaction per unit of charge transfer as:

$$V_{tn} = \frac{\Delta H}{2F} \quad (2)$$

where F is the Faraday constant. For steam electrolysis at standard pressure and a temperature between 600 - 750°C the thermoneutral voltage lies around 1.28-1.29 V.

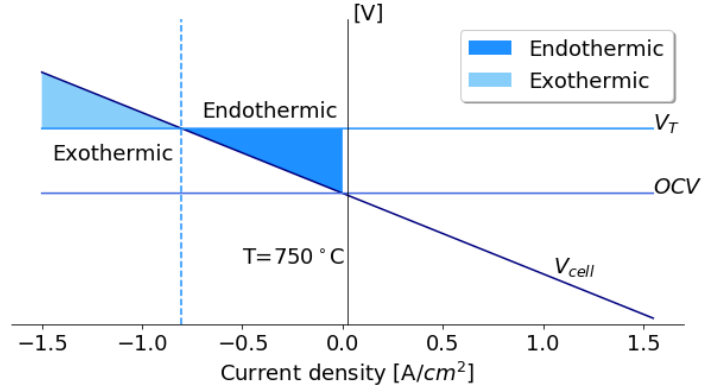


Figure 2: I-V curve for different operational modes showing unique thermal behaviors.

Figure.2 shows a typical current-voltage relation for a given set of operating condition. In the fuel cell mode, the heat generated by the exothermic chemical reaction is higher than the heat removed from the stack as electric power at all current densities. Hence this mode of operation is always associated with net heat generation. In contrast, if the operating voltage of an electrolyzer remains below the thermoneutral voltage, the electrical energy supplied to the stack is lower than the heat required to drive the endothermic electrochemical reaction, thereby leading to net consumption of heat. It is only when the operating voltage exceeds the thermoneutral voltage in the electrolysis mode, the high ohmic contribution results in net heat generation. The striking difference in thermal behavior above and below the thermoneutral voltage is highlighted in Fig. 2. The further the stack operation deviates from thermoneutral condition, enhanced air flow will be required in order to cool down or heat up the stack for conditions above and below the thermoneutral point, respectively²⁸.

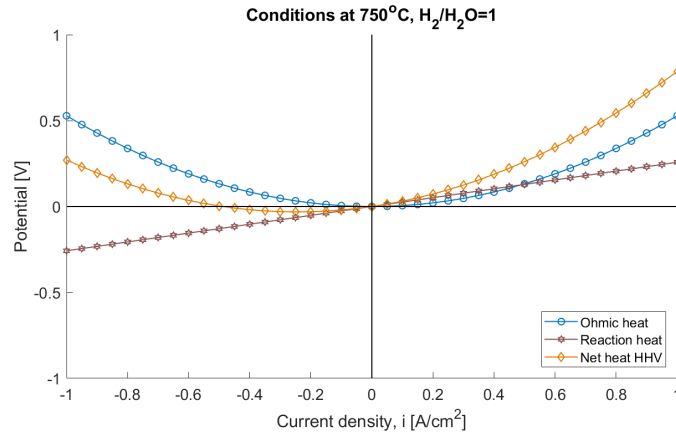


Figure 3: Thermal energy contributions in electrolysis and fuel cell modes.

As the inlet gas mixture proceeds over the cell, its chemical composition changes continuously due to the ongoing chemical reaction. The extent of this chemical reaction depends on several factors, including applied voltage. To further illustrate this, a 1-D model of the cell can be considered as shown in Fig.4 with a segmentations to better visualize how gas mixtures flow from the entry point on the left towards the exit point on the right. Each of the subfigures shown in the Fig.4 represent composition changes over the segments for a certain

voltage condition. The operating voltages are chosen such that they represent situations with voltages below, at, and above the thermoneutral point, covering three main thermal domains of electrolysis mode. Although the initial gas composition is the same in all three cases, the efficiency of steam to H_2 conversion is improved with increasing voltage values. This has a direct consequence on several other cell properties, such as its OCV, current density, net heat output, temperature etc. These changes along the cell are further discussed in Appendix C.

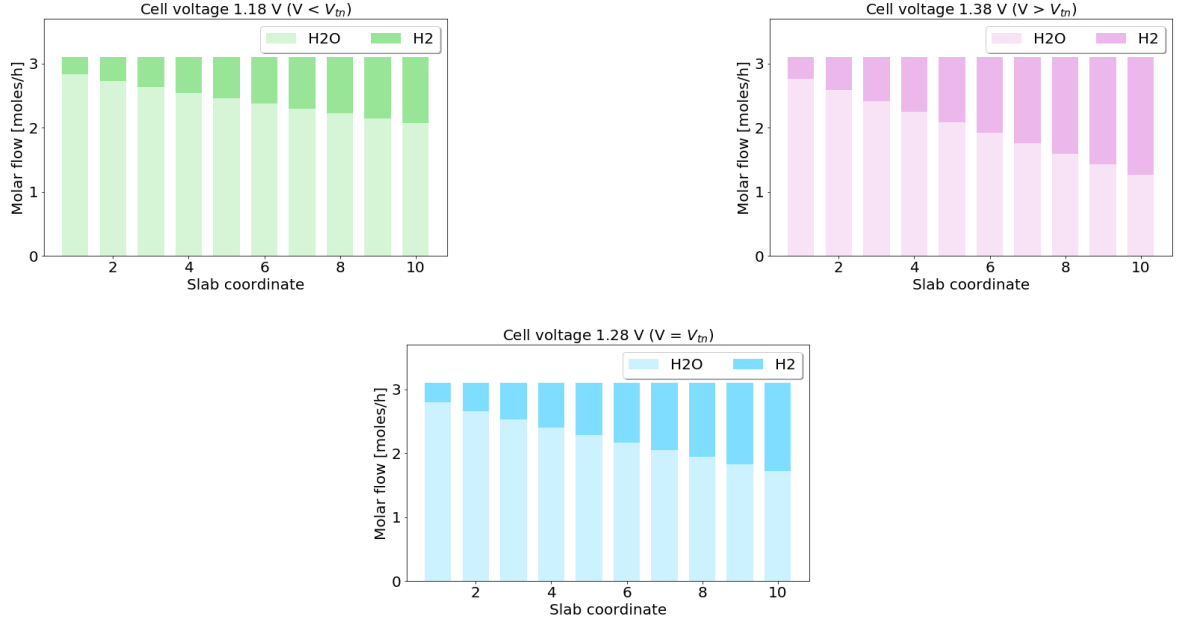


Figure 4: Changes in gas composition through the length of a cell.

While the net heat flux is always positive in the fuel cell mode, it can be either negative or positive or even zero, depending on the operating voltage, in the electrolysis mode. Fig.3 shows the internal heat source and sink terms resulting from the relative contributions of Ohmic and reaction heat. The Ohmic heat source is given by:

$$\dot{q}_{ohm} = i^2 ASR \quad (3)$$

with i being the current density, ASR the area specific resistance. The reaction heat source is given by:

$$\dot{q}_{rxn} = \frac{i}{2F} (|T\Delta S|) \quad (4)$$

where $T\Delta S$ represent the entropy change during the process. The synergies between these two heat sources determines the net heat produced or consumed within the stack. An electrolysis process is inherently endothermic, requiring heat to be provided to drive the chemical reaction in addition to the electrical power. At the same time, heat is also produced within the cell due to internal resistance against current flow. As a combined effect from these two thermal processes, the temperature also changes along the cell. This effect is illustrated in Fig.5 for three different voltage regimes in the electrolysis mode. While temperature remains almost unaffected during thermoneutral operation, it steadily increases in the exothermic mode (voltage above V_{tn}) and decreases in the endothermic mode (voltage below V_{tn}).

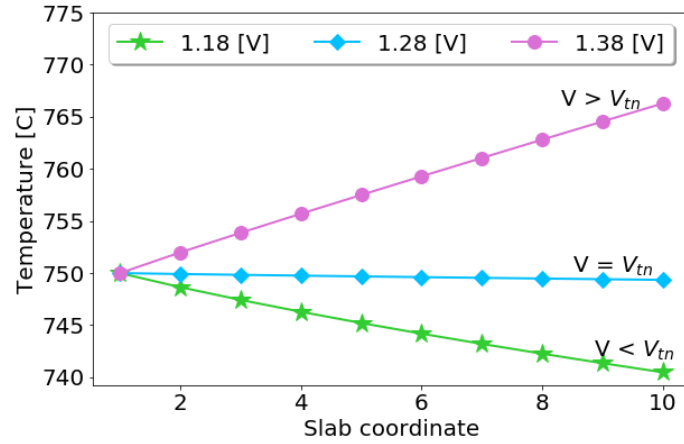


Figure 5: Changes in temperature through the length of a cell.

Although the thermoneutral voltage is strictly a function of temperature only, the net heat source at other operating voltages do however depend on cell ASR and gas composition as well²⁹.

While operating in the thermoneutral mode may seem like an attractive solution in terms of thermal management of the stack, in reality certain flexibilities are demanded for system modulation. Hence, restricting the system to operate only at a specific voltage below thermoneutral is not practically relevant. The voltage should be continuously adjusted as needed for grid balancing. In this case, the system is mainly run in the electrolysis mode with an operating voltage below the thermoneutral point, which ensures net heat is consumed over the cells. This leads to thermal gradients and less beneficial operating temperatures together with larger thermal stresses. In the following section a new operating concept called AC-DC is presented and through the developed model it is demonstrated how this can be used to achieve thermo-neutral operation although the SOEC is operated below the thermoneutral voltage.

For the rest of the time, the system is reversed back to the fuel cell mode, where it is operated to retrieve equivalent amount of heat for the net system to behave thermoneutrally. It is to be emphasized here that this AC-DC method does not change the net heat input to the system, but ensures a rather homogeneous distribution of heat within the stack, which significantly reduces thermo-mechanical stress and improves stack lifetime.

4 Model overview

In order to realize a fossil fuel independent Danish energy system by 2050, the energy scenarios from the International Energy Agency (IEA) suggests that massive changes will be required across all sectors (electricity, heat, transport)³⁰. New emerging technologies are now envisioned to aid in this transition in a cost effective and secure way. In this context, project CORE was proposed to investigate the scope of Power to Gas (P2G) technologies, and to determine how to overcome all existing challenges in order to successfully commercialize this technology. As part of this project, WP2.1 is focused on developing a stand-alone 1-dimensional steady-state SOECⁱⁱ stack model coupled with a simplified implementation of auxiliary components. The model incorporates coupled effects of fluid flow and selective electrochemical reactions on individual electrodes. The aim of this work is to analyze the hydrodynamic and electrochemical properties of a SOEC and to design a operational strategy that will ensure high efficiency of the system.

A conventional SOEC consists of an electrolyte sandwiched between the two porous electrodes, an interconnect for collecting current and supporting stack, and rectangular ducts (channels made of corrugated steel) for the supply of air and fuel. Since SOCs operate at elevated temperature, choosing proper materials for different cell components is crucial to its performance due to additional sensitivity towards thermo-mechanical stress. Several of these cells are arranged up on one another to build the SOC stack. The entire ensemble is well insulated to minimize heat losses and to ensure that the operating temperature is maintained throughout, even if the stack is left idle in between cycles.

Along with the central stack, the model also consists of a number of auxiliary system components, comprising the Balance of Plant (BoP). Main components of BoP include a heat pumps, heat exchangers, water reservoirs, and depending on the down-stream process, a compressor to compress hydrogen gas.

Considering the stack and the BoP components comprising the system of interest, all external factors can be visualized as the ‘environment’ that can be influenced by system’s behavior. This is a crude nomenclature and should not be confused with the thermodynamic definition of system and environment. The environmental modules can be set-up for specific operational schemes. These include a variety of possibilities, such as balancing the surplus and deficit energy in the grid, power arbitrage in the electricity market, modulating the SOEC plant for an AC-DC operation (discussed in Section.3.2) etc. Among all these possibilities, results from three specific test cases are included in the appendix. These are, operating constantly at the thermoneutral voltage thereby ensuring no waste heat is generated, modulating the system continuously to meet balancing demand on the grid, and allowing the electrolysis system to operate close to or below the thermoneutral voltage ($V_{op} \leq V_{tn}$) to occasionally revert to the fuel cell mode to balance the heat energy consumed. In order to calculate how different parameters (such as cell voltage, gas composition, and temperature) evolve along the length of a cell, each cell is divided into segments and a numerical integration scheme is applied to estimate their changes.

The model is developed in Python and the source code will soon be distributed freely under the GNU License agreement, allowing the end users to run, study, modify and share the software, thereby further contributing to the research and development (R&D) of fuel cell

ⁱⁱAlthough the focus here is mainly on the electrolysis mode, it should be remembered that the model can also run in the fuel cell mode, when intended.

community. The principal model comprises of the following sub-models:

- Thermodynamic sub-model (for thermodynamic analysis)
- IV sub-model (for the current-voltage characteristics)
- Operational sub-model (for fluid flow and other operational details)

Further details about each of these sub-models will be available soon in the model documentation.

5 Efficiency expression

Efficiency is a key performance parameter in steam electrolysis. Over the past years, researchers have utilized this to analyze detailed performance, to determine the optimal system design and operational strategies for a cost effective hydrogen production. A number of studies^{5,31} have investigated the thermo-electro-chemical characteristics of high temperature steam electrolysis plants to quantitatively analyze the energy and exergy efficiencies. Mingyi et al.³² made a comprehensive study to determine how the overall efficiency of a high temperature steam electrolysis system is influenced by the a) electrical, b) electrolysis, and c) thermal efficiencies. Their results showed that the contributions were about 70%, 22%, and 8%, respectively. Many researchers have an ongoing effort to integrate SOEC with nuclear and geothermal technologies to optimize the hydrogen production efficiency^{33,34,35,36}. However there are several different expressions of efficiency available in literature, even for the same hydrogen production system. Zhang et al.³⁷ have compared and evaluated three different efficiency expressions for steam electrolysis and proposed different system configurations should be adopted for different operating conditions.

In the most simplest terms, energy efficiency can be defined as the ratio of energy output to that of energy input to a system. In most cases, only electrical energy input is considered in defining efficiency. This can be ambiguous as this may lead to situations of efficiency expressions greater than 100%. In order to avoid this, the efficiency is redefined in this work by considering all energy types that are input to the process. In our case of steam electrolysis, both electrical (E_{el}) and thermal (E_{th}) energies are needed to be provided to produce chemical energy stored in the form of hydrogen, leading to the following efficiency expression:

$$\eta_{LHV} = \frac{\text{LHV}}{E_{el} + E_{th}} \quad (5)$$

where, η_{LHV} is the efficiency, LHV is the lower heating valueⁱⁱⁱ of hydrogen. All terms in both numerator and denominator are expressed on the basis of molar energy (kJ/mole). The relative shares between electrical and thermal energy in the input are mainly determined by system operating conditions. The thermal energy is mostly used to convert liquid water to steam of low/intermediate temperature. This constitutes the following three steps:

$$E_{th} = E_{th_1} + E_{th_2} + E_{th_3} \quad (6)$$

where, E_{th_1} is the heat required to raise temperature of liquid water from storage tank temperature to its boiling point, E_{th_2} is the heat energy needed to water's phase change to vapor state, and E_{th_3} is the rest of the heat available that helps to raise the temperature of water vapor from its boiling point to an intermediate value.

$$\begin{cases} E_{th_1} = nC_p\Delta T & (7) \\ E_{th_2} = n\Delta H_v & (8) \end{cases}$$

$$\begin{cases} E_{th_3} = n \int_{T_1}^{T_2} C_p(T) dT & (9) \end{cases}$$

ⁱⁱⁱEquivalently, higher heating value (HHV) can also be used. Since LHV is normally used in energy system analysis, it is chosen in this work as well.

For 1 mole water at standard atmospheric pressure and tank temperature of 25°C, a total of 55.1 kJ/mole ($E_{th1} = 5.6$ kJ/mole, $E_{th2} = 40.6$ kJ/mole, and $E_{th3} = 8.8$ kJ) heat energy will be needed to raise the final temperature of the steam to 350°C. Notice that the largest contribution to this energy, by far, is in evaporating water from liquid to gas phase.

If the operating voltage of SOEC is maintained at exactly the thermo-neutral point, the thermal energy needed for water splitting precisely balance the Ohmic heat stemming from the internal resistance of the SOEC stack. If the operating voltage is higher than the thermoneutral point, the system appears exothermic in nature, producing more waste heat than needed. On the other hand, if the thermal energy needed is larger than the Ohmic heat, net heat is to be supplied from an external heat source. Hence, presence of a nuclear or geothermal plant in the vicinity can provide high quality waste heat in high temperature water vapor, which in turn result in reduced need of expensive electrical energy.

The gases are cooled as they flow through the stack. Performance analysis is commonly expressed in terms of efficiency (η_{LHV}), where LHV is the Lower Heating Value. Depending on the system considerations, there can be substantial ambiguity in defining exact system efficiency. Zhang et al.,³⁷ have presented a concise collection of different efficiency expressions for SOEC from literature. In this work, we present another efficiency expression which emphasizes on the fact that efficiency is highly sensitive to the availability of steam (instead of liquid water) from any external sources. This expression is shown as:

$$\eta_{LHV} = \frac{\text{LHV}}{E_{total,el} - E_{the}} \quad (10)$$

where $E_{total,el}$ is the total electrical energy input, E_{the} is the externally provided heat (eg., waste heat). The reason for expressing efficiency in this manner is to embed that if waste heat can be utilized then very high efficiencies can be achieved as explained further below. Manufacturers often have the tendency to define total energy input in a single term, without discredmenating between energy sources if supplied internally or externally.

From the perspective of energy balance, production of hydrogen from water electrolysis is given by 242 kJ/mole at 750°C. The input energy in electrolysis comprises of the heating and evaporating liquid water to steam if steam is available ($5.6+40.6 = 46.2$ kJ/mole from above example) to drive the electrochemical reaction in the cell (242 kJ/mole).

To estimate the total energy needed in the process, it is important to know the numerical value of efficiency of current state-of-the-art SOEC stacks. However, such information is often treated as confidential and thereby not available in the public domain. Fortunately, Sunfire, one of the leading manufacturer of SOEC in Germany, has published a system efficiency of 82% in LHV³⁸, corresponding to 3.7 kWh/Nm³ of hydrogen production. Using this realistic estimate of efficiency, one can deduce the total electrical energy input needed for steam electrolysis, which accounts to about 295 kJ/mole. In order to illustrate the effect of externally available heat sources on efficiency, a few examples are discussed below.

Example 1: No external heat source available If all energy is to be supplied electrically, the efficiency drops down to almost 71%:

$$\eta_{LHV} = \frac{242}{(295 + 46) - 0} = 71\% \quad (11)$$

Example 2: Low temperature steam available If an external heat source, such as a geothermal power plant is located nearby, steam can be directly fed into the system, thereby improving its efficiency:

$$\eta_{LHV} = \frac{242}{(295 + 46) - 46} = 82\% \quad (12)$$

Example 3: High temperature steam available In case high temperature steam is available from an external source, efficiency can be enhanced even further. If high temperature steam, e.g. from industrial process, is available at 350°C , E_{th3} will indicate an additional of 8.8 kJ/mole energy compensated (Eq.9), leading to an efficiency around 85%:

$$\eta_{LHV} = \frac{242}{(295 + 46) - (46 + 8.8)} = 85\% \quad (13)$$

These examples emphasize the importance of external heat supplies for an overall improvement in efficiency. Since it has already been pointed out that among all of thermal energy's components, the vaporization stage (E_{th2}) requires the maximum energy input. Once steam is available from external sources, instead of just liquid water, the heat energy demand in the subsequent steps can be significantly small. Even when high temperature steam is available as shown in example 3, the overall improvement in efficiency is only around 3% compared to the low temperature steam case discussed in example 2. The generic efficiency expression given in Eq. 10 can be applied to any system design irrespective of the availability of good quality waste heat. Since SOEC operates at elevated temperatures, utilizing the outlet gas mixture to heat up the incoming steam to further elevate its temperature using a heat exchanger device, one can significantly improve system efficiency.

6 Regulation ability

Integrating large quantities of fluctuating renewable energy sources to the power grid poses serious threat to grid stability issues. To mitigate the frequency deviations (fluctuations) from nominal value in order to constantly maintain power balance in the entire synchronously interconnected system, grid operators use backup reserves with different regulation speeds. In a 2013 report from Aalborg university, Mathiesen et al.³⁹ have projected that for steam electrolysis, SOEC can be ramped to full capacity within 15 minutes in the coming years (2020-2050), with regulation speed of 3 and 0.1% per second for down and up regulations, respectively. If temperature is maintained at desired operating value, fast regulation abilities (within a few seconds) can be expected. But if the operation is started while the stack is in cold condition, it may take around an hour to get it running⁴⁰. The exact time required for such a cold start depends on multiple factors, from design details to material properties in cell fabrication.

Since it is not desired to allow excess waste heat generation within the cell to ensure both performance and longevity of electrodes, SOEC is best applied to operate close to thermoneutral condition. Although this may reflect an ideal strategy, real systems which are connected to the electricity grid require certain flexibility to be modulated to circumvent any deviation in its nominal frequency. Allowing SOEC to have such flexibility, and, at the same time ensuring least waste heat generation, is often regarded as one of the main challenges in optimizing SOEC operations. In this regard, one strategy is proposed here and modeled as part of the *CORE* project.

This strategy takes advantage of the fact that SOEC can be operated in reversible mode with the electrochemistry in the fuel cell mode being exothermic in nature. Although the electrolysis mode is intrinsically endothermic in nature (requires both heat and electricity to be supplied to the system), choosing a voltage lower than the thermo-neutral value can ensure it in cell operation as well. In this way, if the cell is operated in the SOEC mode for e.g., 80% of the time, the rest of the 20% time the mode can be reversed to SOFC to retrieve the heat that is needed for overall balancing.

While adjusting cell voltage in response to available power in the grid (load-following properties) can be achieved almost instantaneously, depending on system design issues remain on fast ramping abilities on the gas-flow side. Fluid flow through a stack to-and-from a pump is affected by numerous factors, including fluid type, length and radius of the pipe and pressure difference across the flow. For all industrial purposes, the flow geometry can be modeled via a simplified flow pattern, without compromising much on the design details. For an incompressible and Newtonian fluid in laminar flow through a cylindrical tube of constant cross section, the Poiseuille's law quantifies how pressure drop may influence the volumetric flow rate. Mathematically expressed:

$$\dot{Y} = \frac{\pi r^4 \Delta P}{8\mu L} \quad (14)$$

where, \dot{Y} is the volumetric flow rate, r and L are the radius and length of the pipe respectively, ΔP is the pressure difference, and μ is the coefficient of viscosity of the fluid of interest.

A crude example of gas flow rate within pipes from the pump to the stack is presented here. For a typical set up of SOEC, let's assume the following:

Reactant utilization factor (μ_f) of 75%

Rate of reactant consumption (\dot{n}_{cons}) 0.029 [mol/s]

Applying Eq. B.8, one can find out the molar flow rate of reactant feed-in: $\dot{n}_{feed} = 0.039$ [mol/s]

Converting to volumetric flow rate, assuming ideal behavior, $\dot{V}_{feed} = 0.003255$ [m³/s].

Assuming a typical pipe of 2 cm radius (cross-sectional area, A of 0.00126 m²) and 3 m length, the velocity (v) of the fluid can be determined as:

$$v = \frac{\dot{V}_{feed}}{A} \quad (15)$$

yielding $v = 2.59$ [m/s]. With this velocity, the gas will require 1.2 second to move through the length of the pipe, which for most practical purposes, can be taken as instantaneous.

7 Economic analysis

To date, the SOEC technology is not yet demonstrated at large scale and is still in the R&D stage. Although several industrial establishments, such as Haldor Topsøe (in collaboration with Risø, DTU), Sunfire, Ceramtec (in collaboration with Idaho National Laboratory), Fuel Cell Energy, HTAS with 300 kW facilities, Bloom Energy with 300 MW installed SOFC capacity in US, have been successful to operate small SOC systems over several thousand hours with flexible operations, the technology has only been demonstrated at max. 185 kW scale (Sunfire methanol production in Dresden). This constitutes a serious challenge when estimating the cost of SOEC systems, as this introduces large uncertainties on the prognosis for large scale production costs. Even with these complexities, SOEC has already identified itself as a promising technology for future power system with large shares of variable renewable energy sources, like solar and wind. Hence, all techno-economic developments of SOEC are projected on a plausible roadmap for the next few decades. From the perspective of CORE project, the advances in the year 2030 are most relevant, but to give our readers an even broader picture, the years 2020 and 2050 are also included here in the discussion.

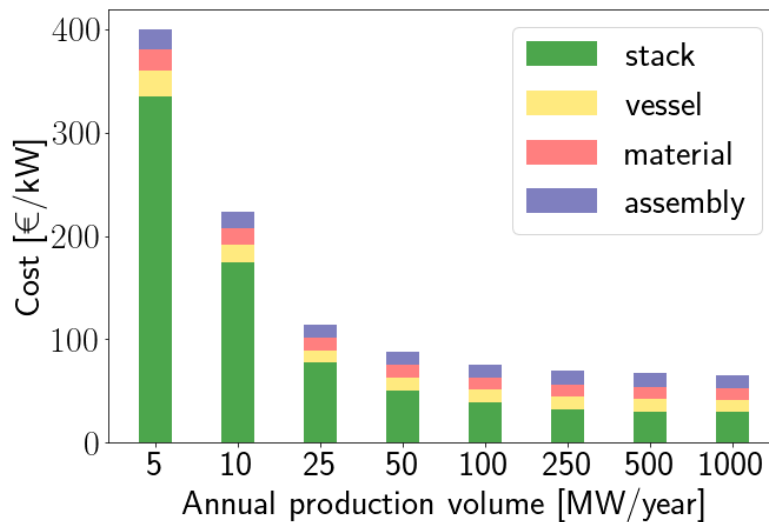


Figure 6: Effect of production volume on estimated manufacturing cost for SOEC stacks with planar rectangular cells, inspired from Jan Thijssen's thesis²⁰.

Among all components of an SOEC system, the most expensive one is the SOEC stack itself. Interestingly enough, not only it is the most expensive one, it also has a much shorter lifetime (around 5 years, as compared to about 20 years for the entire system assemble⁴⁰), causing it to be replaced a few times throughout the entire operating period of the system, and thereby further contributing to the cost. In 2007, Jan Thijssen made an extensive study on the manufacturing cost of SOFCs and reported that stack cost can be reduced almost 4 - 8 times by increasing production volume from 5 - 500 MW/year (per plant)²⁰. According to this work, investment costs are likely to fall in the future due to higher production volume, supply chain development, improvements in manufacturing (increased automation), and technology innovations supporting the competitiveness of SOC against other storage options. It is to be noted here that the Thijssen study estimates all prices for SOFC systems. In this work,

the prices are recalculated for SOEC following the assumption that its rate of cost reduction with increasing production volume is the same as proposed by Thijssen. Due to the internal thermal balancing it is an advantage to operate the SOEC stack at a higher power density than SOFC, thereby resulting in a reduced manufacturing cost for the SOEC systems. To deduce projected SOEC manufacturing cost from the detailed cost calculations for SOFC by Thijssen, a scaling factor of 0.25 is applied here in accordance with the 2013 report from AAU³⁹ and the 2017 report from Energinet⁴¹. Assuming a production volume between 5-10 MW/year in 2020, the SOEC stack price will be between 175-335 €/kW. Following an enhanced mass production of stacks, between 100 and 250 MW/year in 2030 and 2050, the prices will reduce to almost 38 €/kW and 33 €/kW in 2030 and 2050, respectively^{iv}. Fig. 6 is produced following this argument of reduced stack cost in the SOEC mode owing to its higher power density compared to the price projections presented by Jan Thijssen²⁰ for SOFC stacks. Of course, the scaling is also applied on other components shown in Fig. 6, such as assembly, other materials, vessel, and insulation costs, as the costs reflect to the reduced size of the entire ensemble of SOEC. Fig. 6 indicates that the share of stack modules always dominates over other manufacturing costs, although the effect remains exceptionally prominent for production volumes below 10-25 MW/year. It also shows that the impact of cost reduction via increased production volume decreases after 250 MW/year.

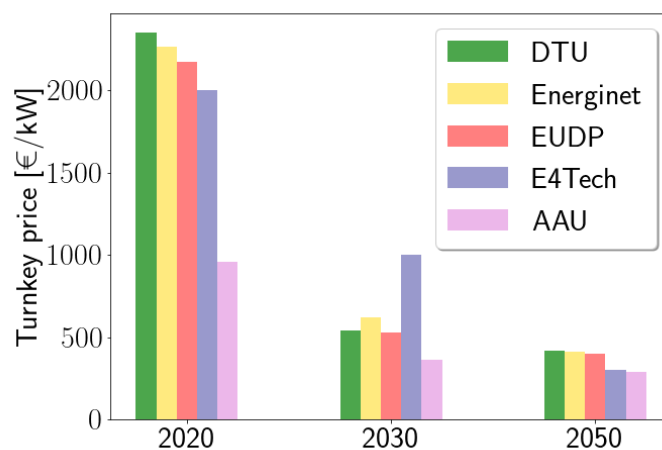


Figure 7: Projected turnkey prices of SOEC for the next decades.

There are several studies in literature from different solid oxide research groups projecting its price for the next decades^{42,41,40,43,39}. Fig. 7 shows such a comparison of SOEC's turnkey prices for 2020, 2030, and 2050. While there is a common trend of cost reduction over time, there is substantial difference in opinion among different research groups on how will this change be manifested in reality. From Fig. 7, it can be seen that some studies like those by E4Tech⁴³ and AAU³⁹ assume a more linear approach, others opt for an exponential fall in prices with time^{42,41,40}. Although most studies are in good agreement for the year 2050, all aiming for a price below 500 €/kW, discrepancies are clear for shorter time horizons. For the intermediate time of 2030, researchers have an array of opinions, from around 360 €/kW projected by AAU to 1000 €/kW by E4Tech. The nearest future, projected via 2020, shows that

^{iv}In a similar assessment by Energinet, the authors have assumed SOEC stack costs of 376 €/kW in 2020, 43 €/kW in 2030, and 36 €/kW in 2050, which are slightly higher than our own calculations⁴¹.

the 2013 report by the Aalborg university was overly optimistic with technology improvement and market integration of SOEC, indicating almost half the price projected by other studies.

Table. 1 summarizes a few key aspects of grid connected SOEC financial data estimated for the upcoming decades, presented in a 2013 report from Aalborg university ³⁹. The calculations in this report are based on the assumption that the costs target factory assembled stacks operating under atmospheric pressure, with stack module costs of 155 €/kW for an annual production volume of 250 MW. They have also identified the additional costs associated with local grid reinforcement to connect electrolyzers to the transmission system. They have also assumed that the fixed operation and maintenance (O&M) costs to be approximately 3% of the annual investments, which in case of 2020 will be 25800 €/MW/year, in 2030 will be 8400 €/MW/year and in 2050 will be 6200 €/MW/year.

		2020	2030	2050
Before grid connection	M€/MW	0.86	0.28	0.21
After grid connection	M€/MW	0.93	0.35	0.28
Fixed O&M	% of inv./year	3	3	3

Table 1: Financial data for SOEC³⁹.

As mentioned earlier, the pre-commercial status of SOC unit induces large uncertainties in its investment costs. Based on literature survey and consultation with the stakeholders, E4Tech has projected commercial SOC unit cost around 2000 €/kW between 2015 and 2020, 1000 €/kW between 2020 and 2030, and only 300 €/kW beyond 2030 ⁴³. The US Department of Energy (DOE) has projected uninstalled capital cost of 727 €/kW for current time and 381 €/kW for future⁴⁴ ^v. In the same report, DOE has provided projection of stack capital cost of 254 €/kW and 88 €/kW for current and future projections, respectively. The E4Tech study defines operational cost (OPEX) to include costs such as planned and unplanned maintenance, as well as overhaul, but not electricity cost. OPEX values are often provided as a percentage of initial capital expenditure (CAPEX). The E4Tech study has suggested OPEX values of 2-5% of CAPEX per year, with no distinction between different technologies. It is important to emphasize here that this figure does not include end-of-life stack replacements.

^vHere a \$ to €- conversion factor of 0.886 is applied as of 04-07-2019.

8 Summary & outlook

Following the immediate consequence of large-scale integration of fluctuating renewable energy sources like wind power to the electricity grid causing large amount of surplus energy in hours of overabundant wind generation with limited power demand, the primary interest of this project report is to assess how power-to-gas technology, such as the state-of-the-art solid oxide cells, can be applied here as a storage device to absorb this excess energy and to maintain grid balance. For this purpose, a 1-D steady state model is developed for the EC mode, but it can be applied to the FC mode as well, if intended. This model is based on the fundamental thermodynamics, electrochemical reactions, gas flow, heat and mass transfer to assess the overall performance and to evaluate thermal and gas balances. The stack model presented here can be applied as a stand alone assessment/design tool, or implemented as a part of an energy system model to allow system studies.

It turns out that stack efficiency can be significantly improved via proper thermal management of the system. This includes choosing a smart operating strategies, such that heat consumed in the electrolysis mode is perfectly balanced by the heat generated in the fuel cell mode, resulting in minimized thermal gradients. Since SOC operates at elevated temperatures, frequent changes in stack's temperature results in the development of thermo-mechanical stress within the stack, thereby diminishing performance and causing rapid degradation.

To overcome this conundrum, stacks can be placed within an insulated environment to avoid frequent cold start-ups and maintaining operating temperature throughout. This may increase the OPEX, but will be beneficial to the lifetime of the SOEC stack. State-of-the-art SOC stacks have a lifetime around 5 years, while the system itself can sustain as long as ~20 years. Since SOC stack is the most expensive component of the entire assembly, its multiple replacements (3-4 times) within system's lifetime induces a major problem, both in terms of economics and technical maintenance. Therefore, improving stack's lifetime by minimizing thermo-mechanical stress is strongly desirable to SOC plant operators. If such plants are connected to the grid, certain flexibility in their modulation is needed, such as ramping up and down on short notice. While adjustment of current and voltage can be made instantaneously, it is shown that gas flow can also be adjusted very quickly, depending on the pressure difference, system design (such as, length and diameter of the pipes) etc.

Given its current price and R&D status, bringing SOC plants onto marketing with highly competitive and well established storage technologies, such as batteries, may seem like a cost intensive outcome. However, SOC plant operators may undertake additional strategies like increasing annual production volume, improving manufacturing, enhancing supply chain developments, selling high purity oxygen (and hydrogen) to chemical industries with large demand for these, taking advantage of electricity arbitrage in the day-ahead and intra-day electricity markets etc., to make it a viable business option. In future, development in material science, innovation in technology supporting competitiveness, sustainable operational strategies, emergence of a fossil fuel neutral energy economy, possible taxation on carbon-based and nuclear power plants, and favorable government policies may further boost development and large-scale integration of SOC plants.

As the project is still ongoing, a few additional features are planned to be implemented in the model in the coming months. These include incorporating co-electrolysis for methanation to improve thermal management and to utilize the existing natural gas grid for storage. The 1-D model can also be either extended to its 3-D form to better understand heat dispersion features within the stack or compare the results of the existing 1-D model with another in-

house 3-D model to identify its lacking features and shortcomings.

Appendices

Appendix A

Thermodynamic background

Calculation of thermal energy needs (thermodynamically represented as $T\Delta S$) and the overall enthalpy (ΔH) can be achieved from standard thermodynamic calculations. In both cases, the estimations can be based on molar heat capacities at constant pressure (C_p):

$$\Delta H_r = \sum_i v_i \times H_{f,i(products)} - \sum_i v_i \times H_{f,i(reactants)} \quad (\text{A.1})$$

$$\Delta S_r = \sum_i v_i \times S_{f,i(products)} - \sum_i v_i \times S_{f,i(reactants)} \quad (\text{A.2})$$

where H_f and S_f are the enthalpy and entropy of formation of each species, respectively and are deduced from the following thermodynamic expressions:

$$H_f = H_f^0 + \int_{T^0}^{T_{op}} C_p dT \quad (\text{A.3})$$

$$S_f = S_f^0 + \int_{T^0}^{T_{op}} C_p \frac{dT}{T} - R \int_{P_0}^{P_{op}} \frac{dP}{P} \quad (\text{A.4})$$

To account for the temperature-dependence of C_p , it is expanded as a polynomial of temperature using a parametric model, proposed by a group of researchers of Cambridge university⁴⁵ and validated against the NIST database (the latter uses a set of parametric equations, known as the Shomate equation, to obtain C_p).

Once ΔH and $T\Delta S$ are obtained from above calculations, changes in Gibbs free energy can be calculated with:

$$\Delta G = \Delta H - T\Delta S \quad (\text{A.5})$$

Appendix B

I-V characteristics

In a fuel cell, the electrical work done by moving a charge on one mole electron through the external circuit is equivalent to its voltage. For an ideal (reversible) process, where there is no losses in the cell, this electrical work done will be equal to the Gibbs free energy released.

$$\Delta G = -2FE \quad (\text{B.1})$$

where F is the Faraday constant and E is the electromotive force or the reversible open circuit voltage. The digit 2 in Eq.B.1 appears due to the exchange of two electrons as given in the Eq.1 above.

From thermodynamics, the Gibbs energy change under non-standard conditions can be related to the Gibbs energy change under standard pressure via:

$$\Delta G = \Delta G^0 + RT \ln \frac{p_{H_2} p_{O_2}^{0.5}}{p_{H_2O}} \quad (\text{B.2})$$

Dividing both sides of Eq.B.2 by $2F$, and substituting by E , one can obtain the Nernst potential (E) as:

$$E = E^0 + \frac{RT}{2F} \ln \frac{p_{H_2} p_{O_2}^{0.5}}{p_{H_2O}} \quad (\text{B.3})$$

E is the theoretical maximum cell potentialⁱ. Actual cell potential is always subjected to certain loss processes, such as activation loss (η_{act}), concentration loss (η_{con}), and Ohmic loss (η_{ohm}) etc. These individual loss processes are well discussed in literature^{37,46}. One of the advantages of SOC modeling is that all these loss processes can be represented using a single quantity, the Area Specific Resistance (ASR), as:

$$ASR = \frac{\eta_{act} + \eta_{con} + \eta_{ohm}}{i} \quad (\text{B.4})$$

where i is the current density. In this work, ASR is derived from curve fitting on a series of measurements on different operating conditions in the Risø National Laboratory of DTU^{7 47}. Considering above loss processes, the cell voltage can simply be expressed as:

$$V_{op} = E - ASR \times i \quad (\text{B.5})$$

ⁱThe voltage E can also be derived directly from Eq.B.1 if ΔG is known from thermodynamics under non-standard conditions.

It is very important to emphasize here that our model assumes that the operation is valid within the linear part of the I-V curve. With known operating voltage, cell power density (pd_{cell}), and hence power itself, can also be derived as:

$$pd_{cell} = V_{op} \times i \quad (B.6)$$

Based on Faraday's laws the molar flows for reactant consumption in each cell is defined as follows:

$$\dot{n}_{cons} = \frac{I}{2F} \quad (B.7)$$

where \dot{n}_{cons} is the molar flow rate and I is the current. During a real operation, a certain fraction (usually around 75-80%) of the reactant fed into the system is converted to products, and the rest comes out unreacted. Applying this reactant utilization factor (μ_f), the molar flow rate of reactant feed can be calculated as:

$$\dot{n}_{feed} = \mu_f \times \dot{n}_{cons} \quad (B.8)$$

It is worth mentioning here that although high reactant utilization factor may seem desirable, very high μ_f values (close to 100%) may cause localized reactant starvation, thereby heavily degrading the performance.

Appendix C

Dynamic changes along the cell

As the inlet gas passes through the cell, its composition changes due to the ongoing electrochemical reaction, which in turn, strongly influences certain other cell parameters. For this purpose, a 1D model is considered where each cell is hypothetically divided into a few segments and the changes in gas flow rate, OCV, current density, Ohmic and reaction heat, and temperature are calculated using an iterative method. Among these parameters, gas flow rate and temperature changes have been already analysed in the main text (Sec.3.2), and therefore will be skipped in the following discussion.

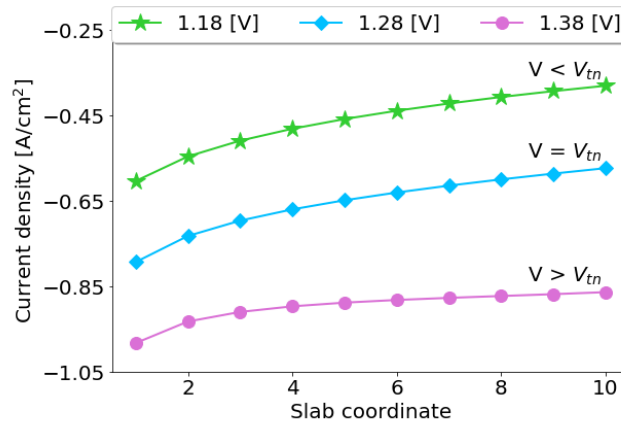


Figure C.1: Changes in current density through the length of a cell.

The effect of changing gas composition can be viewed directly on current flow (or equivalently on current density) via Faraday's law. Fig.C.1 shows the changes in current density as the gas mixture propagates through the segments. This example is drafted exclusively for the operation in the electrolysis mode, hence the negative sign in the current density values. Fig.C.1 also shows that higher operating voltage results in improved electrochemistry, thereby enhancing current flow through the stack.

Gas composition also directly influences the open circuit voltage (OCV). Fig.C.2 outlines an example of electrolysis operation where OCV is shown to increase from the entry to the exit point for three different voltage conditions. These three voltages are chosen such that they represent the three thermal regimes in the electrolysis mode, with operating voltage being at, above, or below the thermoneutral point.

It is discussed in Sec.3.2 that the net heat generation/absorption depends on the synergies

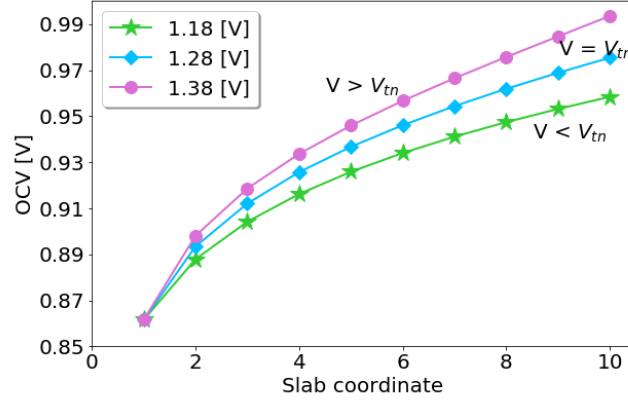


Figure C.2: Changes in OCV through the length of a cell.

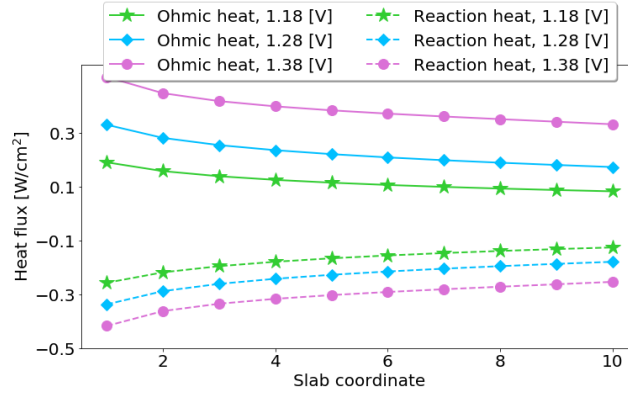


Figure C.3: Changes in Ohmic and reaction heat through the length of a cell.

between Ohmic heat and reaction heat. The reaction heat is endothermic (requires heat to be supplied) in the electrolysis mode and exothermic (heat is produced) in the fuel cell mode. By convention, heat produced is taken as positive and heat removed (or absorbed) as negative. Thus reaction heat can be either positive or negative, depending on the mode of operation. The Ohmic heat, on the other hand, is always positive as it is derived from the resistance against the current flow. Fig.C.3 illustrates the Ohmic and reaction heat changes along the cell during an electrolysis operation. The colors are shown for three voltage regimes and both Ohmic and reaction heat are found to increase with increasing operating voltage.

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