# Determining best values of operational parameters for reversible Solid Oxid Cell Systems

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**Abstract:** Reversible Solid Oxid Cell Systems can operate in the energy system as electrolysis and fuel cell. In this way they can satisfy future needs for energy storage on different levels. This work focuses on the influence of operational parameters on the system efficiency in different flowsheet options. The approach for modelling the system and generating the results is discussed and an outlook for future works is given.

Keywords: Reversible Solid Oxid Cell, Energy storage, Power-to-Fuel, Electrolysis, Fuel cell

#### **1** Introduction and Motivation

In Austria the government declared in the Mission 2030 ambitious plans for increasing mainly renewable electricity production and lowering the emissions of greenhouse gases. Already today our electric energy grid is facing huge challenges regarding the volatile nature of renewable producers like wind turbines and photovoltaic panels. Increasing renewable electricity usage will inevitably require a strengthening of electricity grids as well as novel energy storage solutions and a coupling between different energy carriers. Those storage and coupling systems can be integrated on different levels, from household appliances and industrial systems up to centralized plants at utility scale. A reversible Solid Oxide Cell System together with a hydrogen storage can provide flexibility with different temporal periodicity and scale. Various different ideas for the system configurations already have been proposed in literature by various research groups [1–8]. It is widely agreed that a recirculation on the fuel gas side is advantageous. In our research we are investigating the implications of these different system flowsheets for the efficiency and their suitability for the wide range of applications mentioned before.

# 2 Introduction to reversible Solid Oxide Cell (rSOC) Systems

The rSOC-System under investigation is a based on a high temperature solid oxide cell, which can be operated in fuel cell mode (FC) and electrolysis cell mode (EC). In FC-mode the fluid entering the system is pure hydrogen while in EC-mode it is demineralized water. According to the characteristics of the rSOC-Stack an electrochemical potential difference between  $H_2/H_2O$  and air electrode can be used in an external circuit (FC-mode) or must be overcome (EC-mode) to reverse the reaction. By connecting the rSOC-Stack with components that provide the  $H_2/H_2O$  and air with adequate compositions and temperatures we arrive at the rSOC-System.

The system performance was evaluated on the base of two different flowsheets, cold-gas-recirculation and hot-gas-recirculation, which can be seen in Figure 1.



Figure 1 Basic system flowsheets, A) with hot- and B) with cold-gas-recirculation

The main difference between these configurations is, that with hot-gas-recirculation the ejector is working at the stack temperature and with cold-gas-recirculation the ejector operates closer to the atmospheric boiling point of water. Another interesting observation is that in the electrolysis mode the  $H_2O$  temperature after the evaporator (see the left side of Figure 1) is always higher than the boiling temperature of water. As a result, there cannot occur condensation in the exhaust fuel leaving the heat exchanger ( $H_2/H_2O$  HX). In fuel cell mode there is no such limitation. One identified influencing mechanism for the system efficiency, that can be tuned in a wide range, is connected to the recirculation rate. Increased recirculation leads to a more homogeneous gas composition and temperature in the stack. Additionally, the fuel utilization is raised. On one hand both these effects increase the efficiency but on the other hand higher recirculation lowers the fuel concentration in the stack, which decreases the efficiency. In the flowsheet B) of Figure 1 a condenser in the recirculation is present, which reduces the steam contend in the recirculated stream, and therefore the negative effect of higher recirculation rates is reduced. In the presented research this behaviour and the influence of more parameters on the system efficiency were studied and quantified for various system configurations.

## 3 Methodology and Results

For the investigation of the system performance, thermodynamic steady state simulation models of the system with different flowsheets were set up in Dymola (Modelica Code). The stack behaviour is simulated by a semi-empirical model provided by AVL List GmbH within the project FIRST. The heat exchangers are chosen to be operated in counterflow and the are modelled as 0D objects with a minimum temperature difference in the pinch point ( $\Delta T_{Pinch}$ ). The logarithmic temperature difference and heat exchanger constant are calculated to allow off design-simulation. The models of the evaporator and condenser are assuming that there is a

heat exchange with some not specified environment which allows the working fluid to be heated up above the boiling point or cooled down below the dew point. The temperature for superheating and subcooling ( $\Delta T_{SC}$ ) must be specified and the required or released heat is calculated. The electric heaters (H<sub>2</sub>/H<sub>2</sub>O and Air e-heater) calculate the consumed electric power for heating the H<sub>2</sub>/H<sub>2</sub>O and air stream which is necessary in electrolysis operation to keep the stack temperature (T<sub>stack</sub>) stable.

On the system level additional parameters are necessary to fully specify the problem. The fuel utilization (fu) is defined as the difference between H<sub>2</sub>/H<sub>2</sub>O in- and outflow divided by the inflow of fuel to the system. With stack electric current and fuel utilization the flowrate of the incoming H<sub>2</sub>/H<sub>2</sub>O can be calculated. Furthermore, the recirculation rate (rr) is specifying the ratio of recirculated flow to H<sub>2</sub>/H<sub>2</sub>O inflow in the ejector. Finally, the air excess ratio ( $\lambda$ ) is the ratio of the oxygen flow on the air side and the oxygen flow through the electrolyte of the stack. In FC-mode  $\lambda$  is calculated by the model, so that the temperature during the exothermic operation is stable. It turns out to be always above the minimum value limit, given by the stack reaction oxygen flow. In EC-mode  $\lambda$  can be set almost freely, as the air stream is functioning as purge gas only.

In our simulations we made parameter sweeps in a technically feasible range over the component and system parameters described above. The parameter value range for these sweeps can be seen in Table 1.

| Parameter   | Minimal<br>value | Middle<br>value | Maximal<br>value |
|---|------------------|-----------------|------------------|
| Stack temperature (T <sub>Stack</sub> ) [°C]        | 700              | 750             | 800              |
| Recirculation rate (rr) [-]                         | 0.5              | 2.75            | 5                |
| Fuel utilization (fu) [-]                           | 0.85             | 0.918           | 0.985            |
| Fuel HX ( $\Delta T_{Pinch}$ ) [°C]                 | 5                | 10              | 15               |
| Air HX (EC / FC) ( $\Delta T_{Pinch}$ ) [°C]        | 5 / 70           | 10 / 80         | 15 / 90          |
| Air excess ratio (EC only) ( $\lambda$ ) [-]        | 0.5              | 1.0             | 1.5              |
| Subcooling temp. (FC only) ( $\Delta T_{SC}$ ) [°C] | 50               | 60              | 70               |

Table 1: Parameter variation values

With this set up for the model, the efficiency for the different operation modes referring to different application scenarios can be calculated according to the equations (1)-(4).

$$EC \qquad \qquad \eta_{E,EC} = \frac{P_{fuel}}{P_{Stack} + P_{fan} + P_{e-heater} + Q_{evaporator}}$$
(1)

$$\eta_{E,FC} = \frac{P_{Stack}}{P_{Fuel} + P_{fan}}$$
(2)

$$\sum_{i=1}^{\infty} EC \qquad \qquad \eta_{I,EC} = \frac{P_{fuel}}{P_{Stack} + P_{fan} + P_{e-heater} + Ex_{evaporator}}$$
(3)

$$\eta_{I,FC} = \frac{P_{Stack} + Ex_{air} + Ex_{fuel} + Ex_{Condenser1}}{P_{Fuel} + P_{fan}}$$
(4)

In the energy sector scenario, it is assumed that there are no facilities nearby the rSOCsystem. Therefore, no thermal coupling is possible and the heat demand in the evaporator must be provided electrically (equation (1) and (2)). The industry scenario reflects the application in a system with ideal thermal coupling. In this scenario waste heat is available to cover the evaporator's energy demand in EC-mode and there are consumers for the waste heat of the system in FC-mode. The required and the emitted heat is scaled with a Carnot factor of the ambient and the process temperature. The Exergy values (EX), that are calculated with the Carnot factor, are used in the calculation of the system efficiency (equation (3) and (4)).

Figure 2 shows the dependency of the different efficiencies according to equation (1) to (4) on the change of parameters for the system with the cold-gas-recirculation flowsheet. In EC-mode an increase of all parameters, besides fuel utilization, results in a decrease of the system efficiency. However, in FC-mode an increase in all parameters but the stack temperature increases the efficiency. Another difference between EC- and FC-results is that the overall sensitivity of the efficiency in EC-mode is very small compared to FC-mode. When comparing energy and industry sector it can be noted that there is a noteworthy change of slopes but the overall trends stay the same.



Figure 2 System sensitivity on parameter changes according to Table 1 for the system flowsheet with cold-gas-recirculation

In Figure 3 we can have a closer look into the efficiency pattern in the rr-fu plane. By comparing the results for the efficiency maxima in the energy and industry scenario, we can clearly see, that the thermal coupling in the industry sector can significantly increase the system performance. The shape of the efficiency pattern for EC and FC operation looks significantly different. This is a result of the condenser in the recirculation, which is only active in FC-mode. By removing steam from the recirculated gas in this way, an increase in rr has a solely positive impact on the efficiency. Furthermore, the fuel utilization (fu) can be very high if rr is large.



Figure 3 Dependency of efficiency on the volumetric recirculation rate (rr) and fuel utilization (fu), for the system with cold-gas-recirculation, in energy and industry sector scenario for electrolysis and fuel cell operation mode. The non-allowed stack operation region is the greyed zone above the black line. red dot – efficiency maximum, white dot - efficiency minimum

In a system with hot-gas-recirculation the FC-mode efficiencies with 56% for the energy sector and 64% for the industry sector are significantly lower. This is caused by the lack of the recirculation condenser.

# 4 Conclusions and Outlook

With the described approach the system behaviour was studied in different system configurations. From Figure 2 it can be noted that finding the proper operation parameters is more important in the FC-mode than in EC-mode. The fuel utilization and the recirculation rate have a strong impact on the system performance. Figure 3 allows us to conclude, that high system efficiencies can only be realized if the system allows a high recirculation and fuel utilization rate. This conclusion was also found to be true for the system with hot-gas-recirculation.

Additionally, to the pure hydrogen operation mode, together with Forschung Burgenland, Energie Institut of the JKU and AVL List GmbH, a system capable of running with  $CH_4$  in fuel cell mode is under investigation. The application in buildings, industries and energy networks will be addressed in further studies. The presented model will be used for time series base calculation to simulate the system performance in the real environment of the application scenarios. All these research activities are happening in the context of the FFG funded project FIRST.

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