PERFORMANCE OPTIMIZATION OF SOLID OXIDE FUEL CELL OPERATION WITH ARTIFICIAL INTELLIGENCE

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Abstract: *With their ability to convert chemically bound energy directly into electrical energy, solid oxide fuel cells (SOFCs) are a promising solution to meet the increasing demand for clean and efficient electricity. To accelerate the successful commercialization of this technology, knowledge of the optimal process parameters for efficient, long-term stable and safe operation is of great importance. To reduce the amount of time-consuming and money-consuming experiments required to determine the optimal operating parameters, we used artificial intelligence and combined it with various optimization algorithms to optimize the process parameters of a SOFC. Using a stacked artificial neural network with algorithm-optimized model architecture, we were able to predict the cell voltage of an industrial-scale electrolyte-based SOFC from the cell temperature, gas composition and flow rate on the fuel side, air flow rate, and current. Due to the tremendous prediction speed in the range of milliseconds, a genetic algorithm could be used to optimize the process parameters. The optimization resulted in electric efficiencies >54% and process efficiencies >68% with 80% fuel utilization for operation with methane/steam mixtures and electrical system efficiencies of >66% for operation with hydrogen/steam mixtures and ideal exhaust gas recirculation.*

Key words: *solid oxide fuel cell (SOFC), performance optimization, artificial intelligence (AI)*

1. INTRODUCTION

In this age of climate change and skyrocketing electricity and energy prices, clean, reliable and efficient power generation is of significant importance. High-temperature solid oxide fuel cells (SOFCs) enable the direct conversion of chemically bound energy of gaseous fuels into electricity, without the limitations of Carnot efficiency. SOFCs are thus a technology with great potential to meet this demand for clean and efficient electricity generation. Due to their high operating temperature in the range of 700-1000°C, precious metals such as platinum are not required.

In addition, unlike low-temperature fuel cells, SOFCs can run on a wide range of fuels, including hydrogen, ammonia, and hydrocarbons such as methane, methanol, or even biodiesel. Despite its unique properties and advantages, further research on this technology is needed for successful large-scale commercialization. In particular, knowledge of efficient but long-term stable and safe operating parameters is essential for proper operation on an industrial scale. In order to determine these operating parameters, time-consuming and costly experiments usually have to be performed. The authors of this paper propose a cheaper and faster alternative by using modeling, algorithm-based optimization and artificial intelligence. Several steps were necessary to get optimized operation parameters. In Figure 1 the steps conducted for this work are summarized.

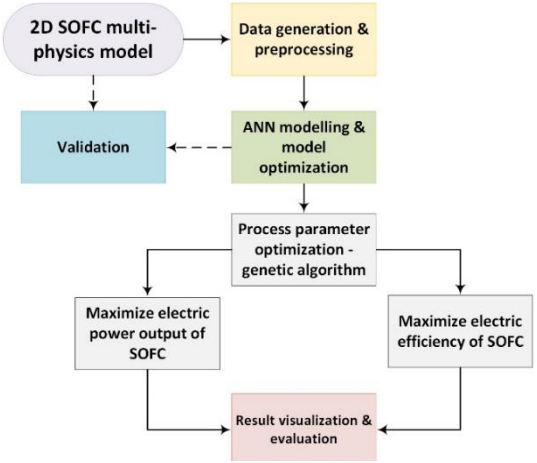

Figure 1: Simplified workflow of SOFC operation parameter optimization

In a first step a multi-physics SOFC model was used to generate a dataset, which represents the whole potential operation range. After preprocessing, this data is used to set up and train an artificial neural network (ANN) model. Both the multi-physics and the ANN model were validated by means of experimental data. The trained and validated ANN model is coupled with a meta-heuristic optimization algorithm (genetic algorithm) to enable a fast optimization of the operation parameters. Following this approach four different scenario cases were investigated:

- Maximum electric efficiency with H_2/H_2O – mixtures as fuel and off-gas recirculation
- Maximum electric power output with H_2/H_2O – mixtures as fuel
- Maximum electric efficiency with CH_4/H_2O – mixtures as fuel
- Maximum electric power output with CH_4/H_2O – mixtures as fuel

2. METHODS

In the following section mainly used methods (see Figure 1) are described more in detail.

2.1 Multi-physics model

To have an as accurate as possible representation of a real SOFC, a 2D multi-physics SOFC model based on more than 120 equations (Subotić et al., 2020), was further enhanced by reaction kinetics (represented by Maier et al., 2011), heat fluxes and local current density distribution (Goodwin et al., 2021). With this complex model the cell voltage, temperature distribution in flow direction, local current density distribution and the magnitude of the ohmic-, activation- and concentration-over potential can be predicted for the cells used. In order to examine the accuracy of the model developed, predictions of the model were compared with measured data from industrial-sized (81 cm² active area) single cell tests. Maximum deviations of 2.1% could be observed. The time required to compute the cell voltage for one operation mode (= temperature, gas composition and current density) with this model is in the range of 2-3 minutes. A direct combination of a multi-physics SOFC model and an optimization algorithm (e.g. a genetic algorithm) therefore might result in an undesired long computation time.

2.2 Artificial neural network model

In order to have a prediction speed, that is fast enough for the coupling with the genetic algorithm, an artificial neural network (ANN) was used in this work. With this meta-model, the cell voltage for a set of input parameters, namely: current density, cell temperature, mass flow rate of H_2, H_2O, CO, CO_2, CH_4 and N_2, could be predicted within milliseconds. To achieve a high model consistency and prediction accuracy, a repeated k-fold cross validation with cyclic learning rate and an algorithm-based hyperparameter-tuner was implemented. These measures led to a negligible additional prediction error of 3mV at maxima, whereby a speed-up by a factor of >3500 compared to the multi-physical model could be achieved. For more details on the specific details of the individual steps interested readers may have a look at (Mütter et al., 2023).

2.3 Genetic algorithm

A genetic algorithm is a meta-heuristic that mimics the process of natural selection and evolution. In general, this algorithm consists of four steps which are repeated until a certain performance criteria or the maximum number of iteration is reached.

- Selection: A population of input parameters is evaluated regarding its "fitness" and only the fittest share is selected to form new a new members of the population.
- Recombination: Pairs from the selected fitter share of the population are recombined to form "parents". These parents combine their features to form new population members until the population limit is reached
- Mutation: Some features of the newly formed population members may be mutated randomly.
- Evaluation: The population is evaluated again regarding its fitness

Due to two different scenarios (CH_4/steam and H_2/steam operation) and two different optimization targets (max. efficiency, max. el. power) per scenario, several different fitness functions were defined.
To maximize the electric power for both CH_4/steam and H_2/steam operation, the fitness function was defined as:

$$Fitness = P_{electric} = Voltage_{cell} \cdot current\ density \quad (1)$$

For the optimization of electric system efficiency of the H_2/steam scenario, the efficiency was defined as:

$$Fitness = \eta_{electric\ sys.} = \frac{P_{electric}}{LHV_{H_2\ processed}} \quad (2)$$

Thereby the unused fuel was assumed to be recirculated with an ideal off-gas recirculation (e.g.: an ejector). For the operation scenario with methane no off-gas circulation was assumed, as its implementation would be much more complex. In order to avoid a CO_2 saturation of the fuel gas, CO_2 would have to be removed from the exhaust gas, which increases system complexity and cost significantly. The electric efficiency for the optimization was defined in a similar way as for the H_2/steam-case as:

$$Fitness = \eta_{electric\ cell.} = \frac{P_{electric}}{LHV_{CH_4\ inlet}} \quad (3)$$

Because the unused fuel can further be utilized, e.g. in gas turbine, in addition to the definition for the fitness function, also only the directly in the SOFC processed fuel was considered for the CH_4/steam efficiency case as process efficiency:

$$\eta_{process\ CH_4/Steam} = \frac{P_{electric}}{LHV_{CH_4\ inlet} \cdot Fuel\ utilization} \quad (4)$$

With the fitness functions defined above, for each scenario and optimization target optimal process parameters were searched. One optimization run thereby required <1h to converge.

3. RESULTS

3.1 Scenario Methane/Steam

For the operation with methane and steam the optimization was facilitated within the boundaries defined in Table 1.

Table 1: Optimization domain and boundary conditions for CH_4/steam scenario.

	Max	Min	Unit
Fuel flow rate	~0.75	~0.32	slpm
S/C-ratio	2	1.5	-
Temperature	805	850	°C
Fuel utilization	80	20	%
Current	90	13	A
Voltage	-	0.65	V

The overall fuel flow rate could be defined at such low rates due to the internal reforming reaction of methane. Through that reaction one mole of methane and one mole of steam are converted to 3 moles of hydrogen and one mole of carbon monoxide (see (5)) and thus increase the overall volumetric fuel flow rate within the fuel cell.

$$CH_4 + H_2O \leftrightarrow CO + 3\,H_2 \quad (5)$$

The Steam/Carbon ratio, which is defined as the molar fluxes of steam over the molar fluxes of all carbonaceous species (in this case only methane):

$$S/C - ratio = \frac{\dot{n}_{steam}}{\dot{n}_{CH_4}} \quad (6)$$

is a metric, which can be used to evaluate the risk of carbon depositions. Those unwanted depositions cause a deactivation of the catalytic active surface of the SOFC and thus should be avoided. The range of the S/C-ratio was defined to stay within safe, yet reasonable operation modes where no carbon deposition may occur. The temperature range was defined in a way, so that the recommended temperature from the cell manufacturer (835°C) lies within the boundaries. Fuel utilization was limited according to manufacturer's recommendation and the current limited based on the capabilities of the in-house available

measurement equipment. Due to potential Ni-reoxidation below 0.65V the cell voltage was limited to values above 0.65V for the optimization.
For the maximum power optimization target, an electric power up to 53.5 W of electric power were suggested by the optimization algorithm. Thereby the following operation conditions were revealed as favourable:

- Maximum possible temperature
- Lowest allowable S/C-ratio
- Maximum possible fuel flow rate
- Highest possible current without violating the lower voltage border

For the maximum power optimization target in the H_2/steam-scenario, the same operation conditions as for the maximum power CH_4/steam scenario were revealed as favourable, whereby an electric power output of up to 60 W could be achieved:

- Maximum possible temperature
- Maximum possible fuel flow rate
- Highest possible current

To have a more realistic system evaluation, thermal losses were also considered for the efficiency evaluation. Overall, the thermal losses were assumed to be 10% of the total thermal energy within the system. These losses were considered by means of a heat exchanger with 90% efficiency. With this added heat exchanger also the pre-heating of fuel and air gas streams, as well as additionally required heating within the oven could be considered.
In Figure 2, the results of the efficiency optimization for the scenario CH_4/steam were visualized in a Sankey diagram. Thereby chemical bound energy is held in blue, thermal bound energy in red and electric energy is coloured in yellow and the following operation parameters and assumptions (marked with *) were used:

Table 2: Input values suggested by optimization algorithm for the CH_4/steam scenario for maximum electric efficiency.

Fuel util.	Temperature	CH4	H2O	Air flow rate	Heat exchanger eff.	El. Power
79%	850°C	0.126 slpm	0.19 slpm	4 slpm	90%*	40.8 W

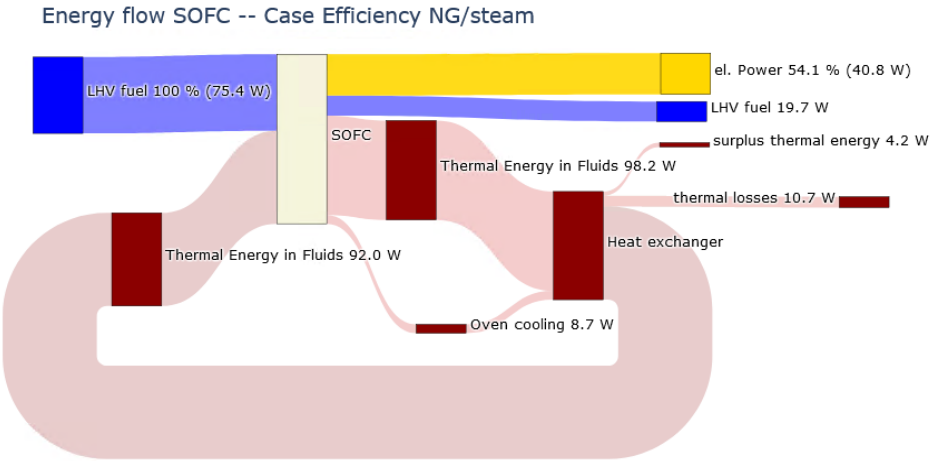

Figure 2: Sankey diagram for optimization target "maximum electric efficiency" for the CH_4/steam scenario. Blue paths represent chemical bound energy, red paths thermal bound energy and the yellow path represents electric energy. Oven cooling was used to close the energy balance.

Without considering the fuel utilization an electric efficiency of 54% could be achieved. Considering the fuel utilization, a process efficiency of up to 68% was observed (see equation (4)).

3.2 Scenario Hydrogen/Steam

For the scenario with only hydrogen and steam as fuel mixture the potential operation range for the optimization can be seen in Table 3.

Table 3: Optimization domain and boundary conditions for H_2/Steam scenario

	Max	Min	Unit
Fuel flow rate	2.437	0.522	slpm
Temperature	805	850	°C
Fuel utilization	80	20	%
Current	90	13	A
Voltage	-	0.65	V

The overall fuel flow rate range was defined with higher boundary values than for the CH_4/steam case due to the missing internal reforming that would have increased the fuel flow rate. For the parameters temperature, fuel utilization, current and voltage the same limitations than for the CH_4/steam case were applied.

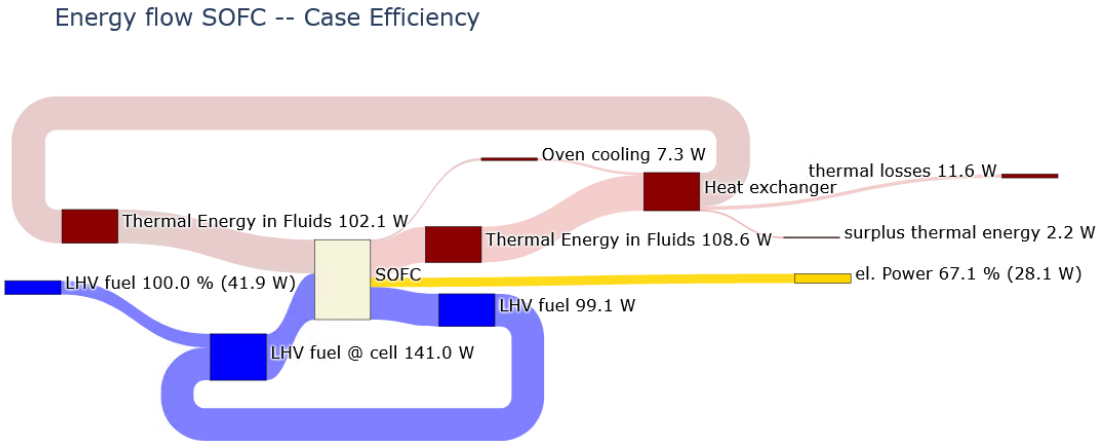

Figure 3: Sankey diagram for optimization target "maximum electric efficiency output" for scenario H_2/steam with off-gas recirculation

In Figure 3 the results of the efficiency optimization for the scenario H_2/steam were visualized in a Sankey diagram. Thereby chemical bound energy is held in blue, thermal bound energy in red and electric energy is coloured in yellow and the following operation parameters
and assumptions (marked with *) were used:

Table 4: Operation parameters for case „maximum electric efficiency" in hydrogen/steam scenario

Fuel util.	Temperature	H2	H2O	Air flow rate	Heat exchanger eff.	El. Power
30%**	850°C	0.784 slpm	0.196 slpm	4 slpm	90%*	28.1 W

** 30% of the total hydrogen supplied to the SOFC is utilized

4. DISCUSSION

4.1 Scenario Methane/Steam

The trends revealed for the maximum power output case can be explained as follows:
With maximum temperature the ionic conductance of the electrolyte is increased and thus the overpotential is reduced. This means that a higher current can be drawn from the cell and thus higher electric power output is achieved. The lowest allowable S/C-ratio leads to the highest possible reactant concentration in the fuel composition and together with higher overall fuel flow rates the chance of local fuel starvations that would lead to higher losses is reduced.
The reason, why maximum possible temperature and lowest allowed S/C-ratio are favourable also for maximum electric efficiency operation can be explained in the same way as for the maximum power case. In contrast to the maximum power case for maximum efficiency the fuel utilization rate is of higher importance. Every unused quantity of fuel has a direct negative influence on the electric efficiency as it increases the denominator in Equation (3) without also increasing the electric power output, leading to a lower electric efficiency. The suggestion of applying the lowest possible overall fuel flow rate can be explained with the reduction of diffusion losses with lower fuel flow rates.

4.2 Scenario Hydrogen/Steam

In contrast to the CH_4/steam scenario, where the algorithm suggested solutions at the lower voltage limit, for the H2/steam scenario solutions with current values at the upper current limit were suggested. This behaviour can be explained by several effects. Firstly, with both H_2 and CO in the fuel mixture the Nernst voltage is lower than with just H_2 in it. Secondly, due to larger molecular size CO may cause higher diffusion losses and thirdly reaction kinetics for the H_2 are faster than for CO.For the maximum electric efficiency optimization target values above 70 % were suggested by the optimization algorithm. These values were only reached when thermal losses were neglected. When considering thermal losses of 10% of the overall thermal bound energy (here modelled as heat exchanger losses) a slight reduction of the overall achievable electric efficiency to around 67 % could be observed (see Figure 3). An explanation for that is that it is more efficient to utilize process heat from the SOFC than to electrically compensate (=heat up) the losses that occur.

5. CONCLUSIONS

The optimization revealed the following main trends regarding desirable operation parameters:

- Maximum temperature for both scenarios (operation with hydrogen and methane) and both max. efficiency and max. power
- Minimum allowable S/C-ratio for CH_4/steam mixtures
- Trade-Off between electric efficiency and electric power output

The highest electric power achieved through the optimization was in scenario H_2/steam with up to 60W for a commercial sized electrolyte supported single cell (126.5cm² active surface area). Electric efficiencies higher than 67% could be achieved for H_2/steam operation when using off-gas recirculating and assuming 10% thermal losses. Operation with CH_4/steam led to slightly lower performance values with ~54W maximum power and 54% electric efficiency at 79% fuel utilization. Thereby it has to be highlighted that no off-gas recirculation was assumed for this case and thus 20% of the reactants are discarded unutilized. When just considering the processed fuel gases a process efficiency of 68% was observed for the CH_4/steam operation scenario. With the method shown in this work, the optimization of the process parameters of industrial-sized solid oxide fuel cells could be carried out with significantly less time and financial effort than if experiments were performed. By using artificial neural networks as a meta-model, the time to predict the voltage for a set of operating parameters was reduced by more than 3500 times compared to the multi-physics model originally used. This speedup enabled the use of a genetic algorithm to optimize the process parameters, which required less than an hour in total to optimize the process parameters for one scenario and one optimization objective, which is significantly less than that required with experiments. With the time and cost reduction achieved, the commercialization of SOFC technology could be significantly accelerated.

6. ACKNOWLEDGMENTS

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