Virtual Fuel Cell System Development with Physics- and Data-Based Models

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Abstract: Fuel cells are once again experiencing an upswing as they are a possible solution for climate-friendly mobility. The aim is to operate them at the highest efficiency, which is highly dependent on the operating condition. In order to run fuel cells at the maximum efficiency continuously, fast-calculating and reliable predictions are essential.

One approach to provide these predictions is artificial neural networks, which are significantly faster in comparison with phenomenological models. In this work, recurrent neural networks are trained with dynamic data of a proton exchange membrane fuel cell. Due to the different time scales of the processes that occur during the operation of the fuel cell, the latest operating state is not sufficient for a precise prediction.

Since, for example, the absorption and release of water in the membrane elapses slowly, the past influences the current prediction. Therefore, the choice fell on recurrent neural networks with long short-term memory cells, which are trained using time series of various dynamic operating cycles. Thus, all time scales are regarded in one combined model that offers fast prediction.

1 Introduction and related Work

Fuel cells (FC) are one of the portable energy supplier technologies for climate-neutral vehicles. Due to the low operating temperature, low operating pressure, compact size, and high power density, proton-exchange membrane (PEM) FC are the most suitable FC technology for individual transportation applications [1]. FCs do not emit any pollutants in contrast to internal combustion engines, since the only product of the reaction in an FC is water. The great benefit of FC electric vehicles (FCEV) over battery electric vehicles (BEV) is the shorter refuelling time. However, the cost of FCs are still high and the hydrogen infrastructure is not well developed yet. Moreover, hydrogen is still expensive which makes it challenging for FCEV to be a serious competitor for BEV as future energy storage technology [2].

To maximize the range of FCEVs, the highest operating efficiency is desired. Two energy management strategies are distinguished: online control strategy and offline control strategy. The latter is a rule-based strategy that optimizes a cost function. For this approach, it is necessary to know the entire driving cycle in advance. By means of the entire cycle, an optimization is conducted. In contrast to this approach, online control strategies are based on real-time controllers and do not require prior knowledge of the cycle. However, it is not ensured that they achieve the global optimum. In this work, a data-based approach is presented, that can facilitate the optimization: due to a very short calculation time, more iteration runs are possible to ensure a global optimum. The basis of the data-based approach are recurrent neural networks (RNN).

Long short-term memory (LSTM) and RNN cells are firmly established for the prediction of fuel cell states in many application scenarios: Pereira et al. [3] introduced an online energy management system for an FCEV that is based on an RNN. It is able to predict the nonlinear dynamics of the FC and achieves higher efficiencies than a heuristic approach. A nonlinear autoregressive neural network for an online energy management strategy is proposed by Zhou et al. [4].

Another application for RNN in the area of FCs is the degradation prediction. Zheng et al. [5] use an RNN with LSTM cells for the performance prediction of a PEMFC under dynamic conditions. Besides the polarization curve, the LSTM network predicts the performance degradation of the FC. A novel model called navigation sequence driven LSTM is proposed by Wang et al. [6], which is an advancement of standard LSTM in order to break the historical degradation data limitations.

In this work, a physics-based 0d/1d simulation model of a 6 kW FC system is set up. With the simulation model random dynamic scenarios are created. The results are taken as training data for a neural networks with LSTM cells. The neural network predicts characteristic operating conditions at the FC stack. The development of this methodology is part of the research project "Development Platform 4.0" ("Entwicklungsplattform 4.0") [7]. In this project, a wide and universal development platform is introduced that is supported by diverse artificial intelligence (AI) techniques. The basis of the platform is a data management system that connects measurement with simulation tools.

The remainder of this article is structured as follows: Firstly, a general overview of the design process of a fuel cell system is given. In the following paragraphs, the physics-based model of the FC system is presented, followed by a description of the data-based model. The results are presented and discussed afterwards, and the paper is rounded off with a short summary and brief outlook.

2 Design Process of a Fuel Cell System

The range capacity and maximum power are two specifications that determine the design of a powertrain system significantly. In the case of an FCEV, both the battery and the fuel cell system determine the amount of storable energy and maximum power supply. Two extreme scenarios are possible: a small FC and hydrogen tank that act like a range extender for a large battery or a large FC system that is only supported by the power of the battery during extreme dynamic power demands. Batteries and fuel cells have different advantages, that need to be combined ideally. For example, a battery has superior transient behaviour, the hydrogen refuelling process is faster and hydrogen has a higher energy density.

The selection of the battery and fuel cell system sizes is the first step when designing a powertrain system (FCEV concept selection). In the next step, the FCEV operating strategy is specified. Precisely, this means that the power split between the two components is defined depending on the power demand, battery state of charge, dynamics, temperatures, etc.. The FCEV operating strategy influences the system efficiency and FC degradation. High dynamics and power demands favour degradation processes. They are also the main factor for the selection of the FC stack size (FC Stack conception). Besides the stack size, also the compressor size and power, the dimensions of the humidifier and the dimensioning of the cooling system play a big role for enabling a reliable and efficient operation. Once the system is defined and the power demand is known, a FC Stack operating strategy must be developed. The aim of the strategy is to optimize the net efficiency of the system for a given power demand while avoiding operation conditions that favour stack degradation. The hydrogen pressure and the hydrogen mass flow rate determine the conditions at the anode side of the stack. They are controlled by the hydrogen inlet valve, hydrogen recirculation blower and purge valve. At the cathode side, the humidifier, the compressor and exhaust valve are set to match a target oxygen pressure and air inlet humidity. Power consumers such as compressor and hydrogen recirculation blower reduce the net power of the FC system. However, a higher oxygen and hydrogen pressure generally increase the efficiency of the FC stack. This is one example of the difficulty to optimize the operating strategy of the FC system.

The iterative process of the design phase of a FCEV is sketched in Figure 1. It demonstrates that a large number of tests and simulations are essential to ensure an efficient and reliable system. Therefore, in the next section, data driven models are introduced as a fast calculating alternative for physics-based simulations.

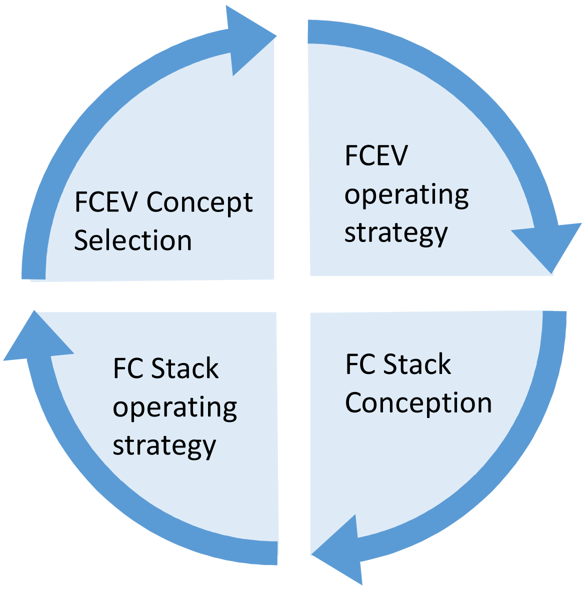

Figure 1: Iterative Fuel Cell System Design

3 Fuel Cell System Models

3.1 Physics-based Model and Data Generation

The examined FC system consists of the FC stack, the air path and the hydrogen path and is schematically visualized in Figure 2. An electrical compressor ensures that enough oxygen is available at the cathode and an additional exhaust valve controls the gas pressure. Additionally, fresh air is humidified externally, if needed. The hydrogen flow is controlled by an expansion valve between the 700 bar hydrogen tank and the FC stack. The hydrogen recirculation blower leads back unused hydrogen. For simplicity, cooling components are not considered. The exemplary FC in this work has a net power of 6 kW.

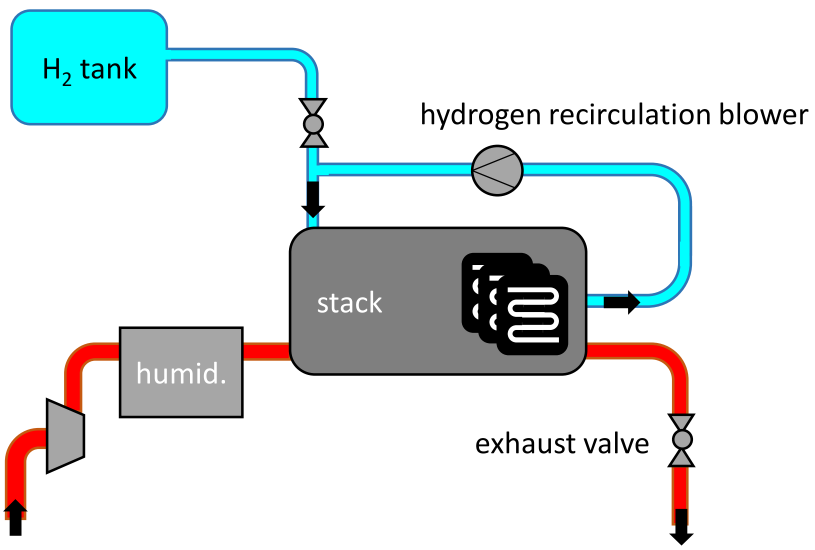

Figure 2: Schematic drawing of the fuel cell system; blue: Hydrogen path; red: Air path

At first, this system is modeled with the 0d/1d simulation software GT-Power. The results are used for the development of the data-based model described in section 3.2. In order to get the ability to predict the fuel cell states in a wide operating range, the training data for the data-based model requires a large variance. To achieve this variance, during the data generation process, the parameters are varied independently of each other. This causes some operating conditions, in which the FC stack is not able to deliver the requested current due to a lack of reactants. In these cases the voltage drops to a minimum level.

During a transient simulation, the following parameters are varied: compressor voltage, humidifier valve position, exhaust valve position, anode target pressure, hydrogen recirculation blower power, current, cooling temperature.

3.2 Data-based Model

Hochreiter and Schmidhuber first proposed long short-term memory cells (LSTM) [8] in neural networks. Nowadays they are a well-established method to predict fuel cell conditions in numerous applications. In this work, the data driven model consists of LSTM cells trained by time series data of the previously described physical model. Since a lot of background information is required for the explanation of the entire creation process, only a brief overview shall be given at this point.

The memory ability of the LSTM cells pave the way for the integration of effects with larger time scales as thermal processes, mass transport delay and diffusion processes. For higher flexibility, separate submodels for the air path and the hydrogen path are created to determine the conditions at the stack's cathode respectively anode. Their prediction is used as feature values for the submodel of the FC stack. Depending on the target and operation purpose of the models, feature and target values are chosen. The neural networks have one input layer, two or three LSTM layers and a fully connected output layer. The exact architectures of the data-based models (number of layers and number of cells per layer) strongly depend on the field of application of the predicting network. As the explained models aim to support the optimization of the control strategy, the feature values are controllable parameters (e.g. compressor power, FC current) and ambient conditions (ambient temperature). The demanded power output of the system is calculated by means of the current and the predicted FC voltage. The target values are the FC stack conditions that give a prediction of the optimization targets (e.g. efficiency). During the training process of the neural networks, the weights between single cells are adopted by the so called ADAM optimizer [9] until the calculated output values match the given target values. The mean average error (MAE) is calculated for the test data at the end of the training in order to get a performance value of a training run.

4 Comparison of the Models

The calculated temporal evolvement of the mass flow rate and the pressure at the stack cathode are plotted in Figure 3 for the physics-based model and the data-based model of a random test scenario. The predicted values act as the feature values for the submodel of the FC stack. The test data, whose results are shown, is not used during the training process. Thus, it is not possible that the neural network does only match the training data und the results are suitable for assessing the generalization quality of the data-based model.

Over all test data, the mean average error (MAE) is 0.013 bar for the cathode pressure and 0.084 g/s for the air mass flow rate. Assessing the time series with the deviation at every time step, the error can have two roots. Either, the calculation of the target based on the features itself is inexact, or the time dependency is resolved inaccurately.

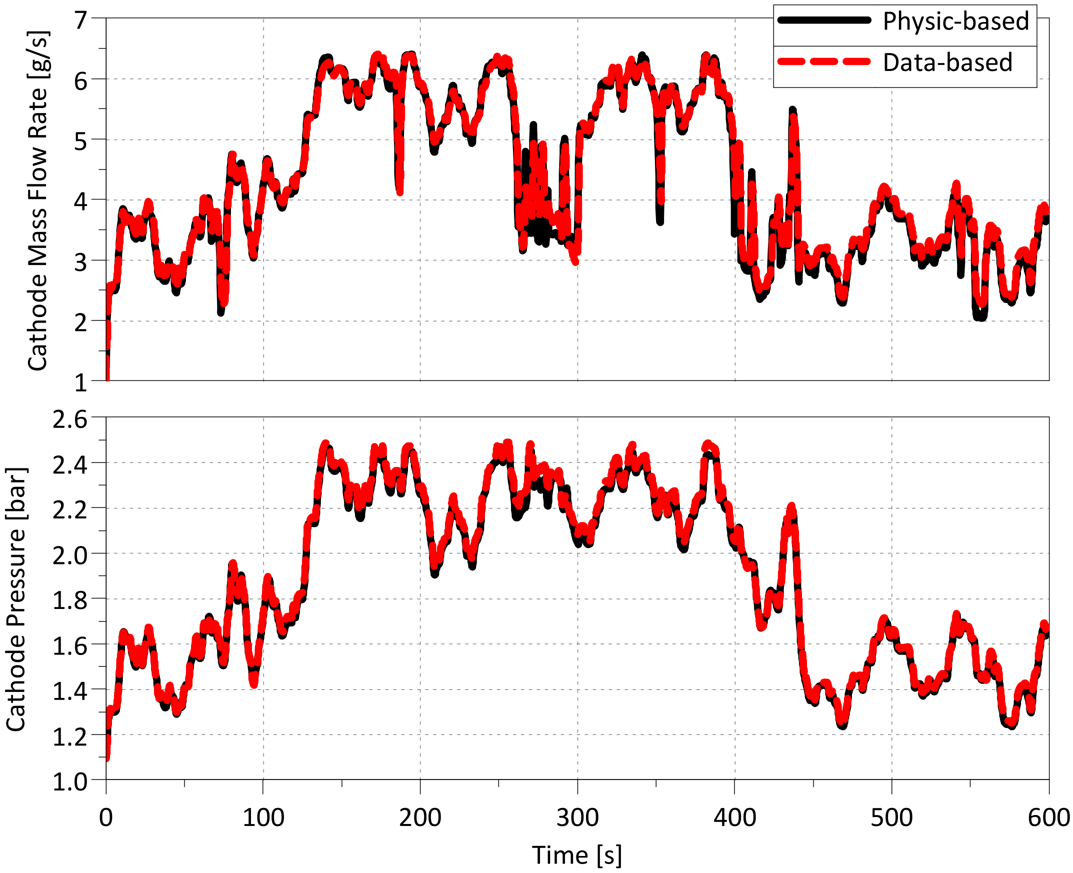

Figure 3: Characteristic result values of the cathode submodel of the physics-based and the data-based model

Similarly, Figure 4 demonstrates the results of the submodel for the FC stack. The provided electrical power of the FC stack is plotted for the physics-based model and the data-based neural network. The MAE is 0.166 kW. Compared to the previous shown results of the air path, the error is slightly higher. The main reason for the larger error, are the points where the drawn current is too high for the conditions at the FC stack. Either the hydrogen, or the oxygen partial pressures are too low for a stable operation. This causes a drop in voltage and power and – in a real fuel cell stack – non-reversible damage is very probable. Between 240 s and 290 s such a state sets in. Not only the physics-based model, but also the data-based model indicate the power drop. The largest deviations are visible, when the power has a short peak after it rises from 0 kW. However, it is not clear, how a real FC stack would behave since damage is likely, as mentioned.

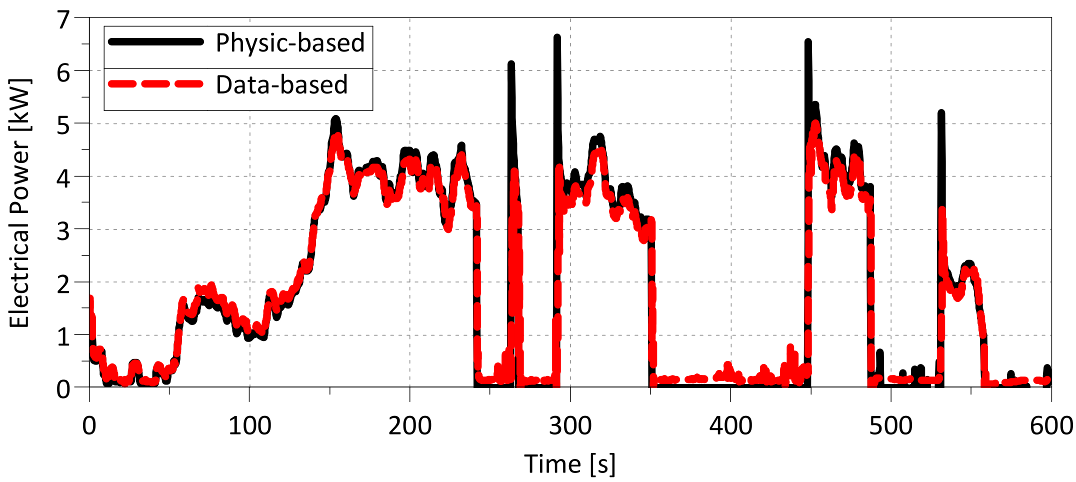

Figure 4: Predicted electrical power by the physics-based and the data-based model

The greatest advantage of the data-based model is the short calculation time. The model predicts the target values more than 100 times faster than real time. In contrast to this, the physics-based model requires approximately 50 times as long as real time and 5000 times longer than the data-based model. Since the data-based models have the possibility to be deployed on several cores in parallel without additional licensing costs, the number of possible runs in a given time is increasable. This enables various application fields for the data-based models: virtual pre-application, dimensioning of components, functional development, model-based controllers, reinforcement learning, application on control units and plausibilization of measurement data.

However, the data-based models only predict the target values for which they were trained. No other values are calculated, unless they are added to the training data. If a detailed result is desired, the physics-based simulation has advantages. Similarly, the data based model can only repeat effects that are present in the training data and they have to be set up in a proper manner for the prediction of a certain effect.

5 Conclusion

A physics-based 0d/1d simulation model of a 6 kW fuel cell system is set up in order to develop an operation strategy. Target of the operation strategy is to optimize the efficiency and reduce degradation during dynamic operation. Due to the large amount of required simulation runs during the optimization process, a fast running data-based model in the form of a neural network with LSTM cells is set up. The needed time series for the training of the neural network is generated by means of the 0d/1d simulation model. The developed data-based neural networks have a up to a 5000 times shorter calculation time compared to the detailed simulation model. It is shown, that despite the drastic reduction of computation time, a high accuracy is maintained. This is beneficial for the offline optimization of the FC control system because many possible system applications are evaluated quickly. It is also possible to implement the data-based model directly on the fuel cell control unit (FCCU) and perform an online optimization. Dependent on the desired purpose, the architecture, inputs and targets of the neural network are adopted.

Reference List

[1] Larminie, J. and Dicks, A., “Fuel cell systems explained,” 2nd ed., Wiley, Chichester, ISBN 0-470-84857-X, 2003.

[2] Sulaiman, N., Hannan, M.A., Mohamed, A., Majlan, E.H. et al., “A review on energy management system for fuel cell hybrid electric vehicle: Issues and challenges,” *Renewable and Sustainable Energy Reviews* 52:802–814, 2015, doi:10.1016/j.rser.2015.07.132.

[3] Pereira, D.F., Da Lopes, F.C., and Watanabe, E.H., “Nonlinear Model Predictive Control for the Energy Management of Fuel Cell Hybrid Electric Vehicles in Real Time,” *IEEE Trans. Ind. Electron.* 68(4):3213–3223, 2021, doi:10.1109/TIE.2020.2979528.

[4] Zhou, D., Gao, F., Ravey, A., Al-Durra, A. et al., “Online energy management strategy of fuel cell hybrid electric vehicles based on time series prediction,” *2017 IEEE Transportation Electrification Conference and Expo (ITEC)*, 2017 IEEE Transportation Electrification Conference and Expo (ITEC), Chicago, IL, USA, 22.06.2017 - 24.06.2017, IEEE, ISBN 978-1-5090-3953-1:113–118, 2017 - 2017.

[5] Zheng, L., Hou, Y., Zhang, T., and Pan, X., “Performance prediction of fuel cells using long short-term memory recurrent neural network,” *Int J Energy Res* 45(6):9141–9161, 2021, doi:10.1002/er.6443.

[6] Wang, C., Li, Z., Outbib, R., Dou, M. et al., “A novel long short-term memory networks-based data-driven prognostic strategy for proton exchange membrane fuel cells,” *International Journal of Hydrogen Energy* 47(18):10395–10408, 2022, doi:10.1016/j.ijhydene.2022.01.121.

[7] “Entwicklungsplattform 4.0,” https//www.ep40.de.

[8] Hochreiter, S. and Schmidhuber, J., “Long short-term memory,” *Neural computation* 9(8):1735–1780, 1997, doi:10.1162/neco.1997.9.8.1735.

[9] Kingma, D.P. and Ba, J., “Adam: A Method for Stochastic Optimization,” 2014, doi:10.48550/ARXIV.1412.6980.