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Short communication

Dynamic fuel cell stack model for real-time simulation based on system identification

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Abstract

The authors have been developing an empirical mathematical model to predict the dynamic behaviour of a polymer electrolyte membrane fuel cell (PEMFC) stack. Today there is a great number of models, describing steady-state behaviour of fuel cells by estimating the equilibrium voltage for a certain set of operating parameters, but models capable of predicting the transient process between two steady-state points are rare. However, in automotive applications round about 80% of operating situations are dynamic. To improve the reliability of fuel cell systems by model-based control for real-time simulation dynamic fuel cell stack model is needed. Physical motivated models, described by differential equations, usually are complex and need a lot of computing time. To meet the real-time capability the focus is set on empirical models. Fuel cells are highly nonlinear systems, so often used auto-regressive (AR), output-error (OE) or Box-Jenkins (BJ) models do not accomplish satisfying accuracy. Best results are achieved by splitting the behaviour into a nonlinear static and a linear dynamic subsystem, a so-called Uryson-Model. For system identification and model validation load steps with different amplitudes are applied to the fuel cell stack at various operation points and the voltage response is recorded. The presented model is implemented in MATLAB environment and has a computing time of less than 1 ms per step on a standard desktop computer with a 2.8 MHz CPU and 504 MB RAM. Lab tests are carried out at DaimlerChrysler R&D Centre with DaimlerChrysler PEMFC hardware and a good agreement is found between model simulations and lab tests.

Keywords: Polymer electrolyte membrane fuel cell; Dynamic model; System identification

1. Introduction

Vehicle operation is likely to be the most demanding fuel cell application. Whereas, the internal combustion engine had more than 100 years to meet today's requirements, fuel cells are forced to catch up within a few decades. The main requirements are high volumetric and gravimetric power density, reliable operation, long lifetimes, low costs and an excellent dynamic behaviour, which in total ties a heavy package for fuel cell research.

Due to their good dynamic behaviour, high power density, compact design, non-corrosive electrolyte, simple manufacturing and a low operation temperature PEMFC are predestined for vehicle applications. In automotive applications round about 80% of operating situations are dynamic. For further development and optimisation of the fuel cell-based power train, models simulating the dynamic behaviour of the system, are of major importance.

In transport applications another model requirement appears. Beside describing the dynamics, fuel cell models implemented in vehicle controller units must be able to do precise simulations in real-time.

From the theoretical point of view, the voltage of a PEMFC stack is a nonlinear multiple input single output (MISO) system. The most important variable inputs are the drawn current, fuel cell stack temperature, pressure, gas composition and humidity at cathode and anode side. For this kind of MISO system, yet there is no standardized procedure neither to find a matching model structure nor to choose suitable types of models.

To meet the requirements the focus is set on black-box models because physical and physically motivated models like Refs. [1] or [2] need a lot of computing time (1 h per step at Intel Xeon 2.0 GHz [1], (100-fold real-time [2]). Unlike physical approaches another advantage of black-box modelling is the capability to identify system parameters with measured data. Using system identification there is no need to know

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specialized material properties like, e.g. pore size distribution of the gas distribution layer or effective active catalyst area.

Applying a systematical process to system identification seems reasonable. The process described in Ref. [3] can be seen in Fig. 1.

Starting with some expert knowledge on the desired system, first a sufficient number of experiments have to be designed. Mainly, there are statistical and conventional approaches for designing experiments. The pros and cons can be read in Ref. [4]. Common in most design methods the investigation boundaries have to be specified. Some are based on system physics, others caused by hardware limiting or safety requirements, respectively. After this step the desired data has to be examined. The quality of the received data will strongly influence the model goodness, so the experimental work has to be done conscientiously. In most cases a post-processing like excepting outliers or some signal filtering of the raw data needs to be done for further analysis. If the resulting data does not satisfy all quality goals some details of the experimental design should be improved and the following steps must be redone. With high quality data a matching model structure has to be selected. One key to succeed in system identification based on modelling is to choose an appropriate model type. In the following step the model parameters have to be identified. The least squares method is the most used parameter identification technique [20]. After the identification step, simulations with the developed model of the desired system behaviour can be done and compared to the measured data. If the gap between simulated and measured data is within acceptable limits, a validation should be done. For validation it is important to use a data record, which was not used for parameter identification [3]. If the model does not agree sufficiently with the observed data or is not good enough for the proposed application another iteration beginning with the model selection step must be applied. Can the questions be affirmed, the model is ready for application.

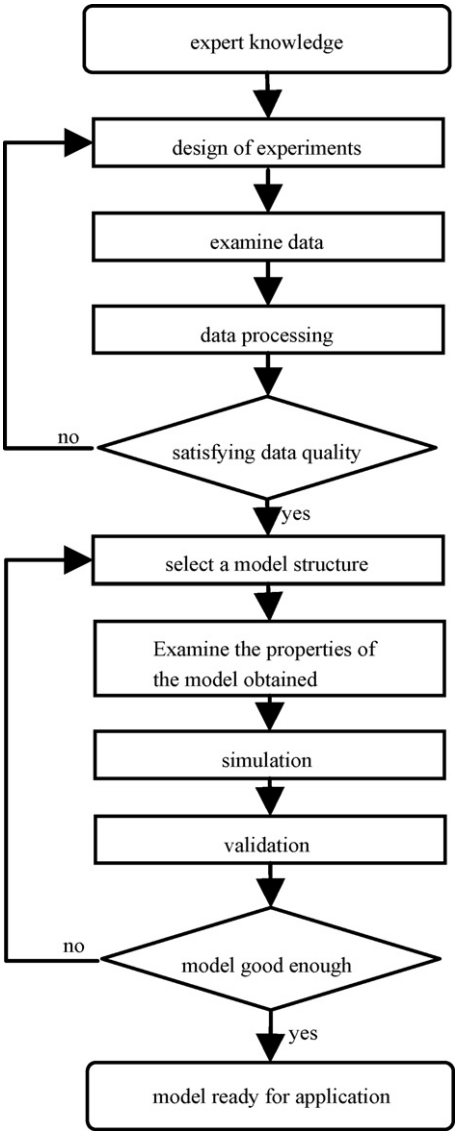

Fig. 1. System identification procedure [3].

Today modern computing technologies offer various supports to handle the model selection, parameter identification as well as simulations with the developed model. In these work packages the presented work was supported by the widespread mathematical software package MATLAB®, provided by The MathWorks Inc.

2. Experimental work

2.1. Design of experiments

A conventional design of experiments (DOE) was chosen due to low knowledge of the dynamic behaviour of the fuel cell stack.

The investigation of the static behaviour of the PEMFC stack was done at five different current densities (i), three cathode excess ratios (λ_c = ratio of oxygen supplied to oxygen reacted), three cathode pressures (P_c) and three relative humidity levels (rh). The anode pressure was adjusted to cathode pressure with a constant offset and anode excess ratio was kept at a constant level as well as the fuel cell stack temperature. To keep the experimental effort acceptable, relative humidity levels at anode and cathode were set equal. This leads to 135 measuring points.

Current dynamics were stimulated by applying positive as well as negative current steps each with four different amplitudes at the same operating point as in case of statically characterization.

Cathode pressure dynamics were also investigated by applying pressure steps. In this case transmembrane pressure difference has to be limited. This limit depends primarily on mechanical properties of the MEA and flow field geometry [5]. Cathode pressure steps were applied only with one amplitude both in positive as in negative direction related to anode pressure level. Therefore, four different steps were investigated.

2.2. Data examination

All experimental work was done with DaimlerChrysler lab hardware. The investigated stack consists of four cells and was operated with pure hydrogen as anode gas and cleaned air as cathode gas. Both reactants were supplied via labora-

tory infrastructure and flow was controlled by digital mass flow controllers. Humidification with deionised water took place in heated trickle beds installed in front of the fuel cell stack. Pressure adjustment of anode and cathode gas was realised by digital controlled valves connected to the air outlet and hydrogen outlet, respectively. Deionised water was used as coolant. Temperature was controlled by matching the coolant flow by controlling the coolant pump speed. Cathode and anode current collector plates were connected to an electronic load via 1 in. wires. Parallel to standard data acquisition with a sample rate of 1 Hz provided by the test bench fast data acquisition was done with a National Instruments PCI DAQ card at a sampling rate of 5000 Hz. Test bench operation was controlled by a standard desktop computer with National Instruments LabVIEW software.

To ensure comparable experimental setup several important parameters were measured. Six thermocouples and pressure sensors were used to measure in- and outlet temperatures and pressures of cathode, anode and coolant flow. Temperature sensors were also placed in the humidifiers to guarantee constant moisture levels.

Measuring the 135 statically points first the current density, cathode pressure and excess ratio as well as relative humidity were set to the desired levels and kept constant for 30 min to reach acceptable steady-state conditions. Some quality control about reaching steady-state conditions was done by viewing the stack voltage time plot. After this 30 min a 2 min mean with a resolution of 1 measurement per second was taken for steady-state value.

Transient voltage behaviour during current variation was characterized by standard resolution of 1 Hz over a long time period and to get better information about fast current dynamics for one second stack voltage was measured with a sampling rate of 5000 Hz additionally.

The response on pressure steps were mapped again with 1 Hz.

To avoid degradation influence in the recorded data in regular time intervals reference VI-characteristics were taken and compared to begin of test campaign VI-characteristics.

Finally, the time elapsed from start to end of simulation was measured with a standard watch.

3. Fuel cell stack model

System theory provides numerous classes of models each with benefits and disadvantages. A brief overview on classes of system models is given in Fig. 2.

3.1. Model structure

To meet the real-time capability the focus is set on empirical models. Fuel cells are highly nonlinear systems [7], so often used auto-regressive (AR), output-error (OE) or Box-Jenkins (BJ) models accomplish no satisfying accuracy. Best results are achieved by splitting the behaviour into a nonlinear static and a linear dynamic subsystem, a so-called Uryson-Model [6].

Fig. 3 shows the developed model structure.

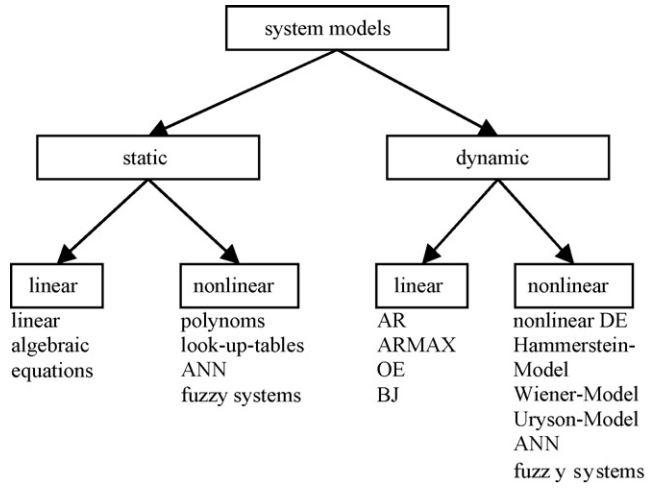

Fig. 2. A brief overview on classes of system models (ARMAX, auto-regressive moving average model with exogenous inputs; DE, differential equation; ANN, artificial neuronal network) [6].

3.2. Nonlinear static subsystem

There are a lot of publications about steady-state behaviour of PEMFC [7–14].

In this work the focus is set on a dynamic fuel cell stack model for real-time simulations. Therefore, an easy to handle and very precise element for the nonlinear static subsystem is desired. Look-up-tables combine these attributes in the most efficient way [21].

The empty spaces between the 135 measured points were bridged by spline interpolation. In the investigated operating area the error between the look-up-table data and the measured stack voltages is below 60 mV, so the look-up-table can be considered as precise.

The disadvantage of this method is the relatively great effort. If more than four inputs should be varied over a wide range the look-up-table method reaches an enormous number of experiments (e.g. 7 inputs each with 4 levels lead to $4^7 = 16{,}384$ experiments!).

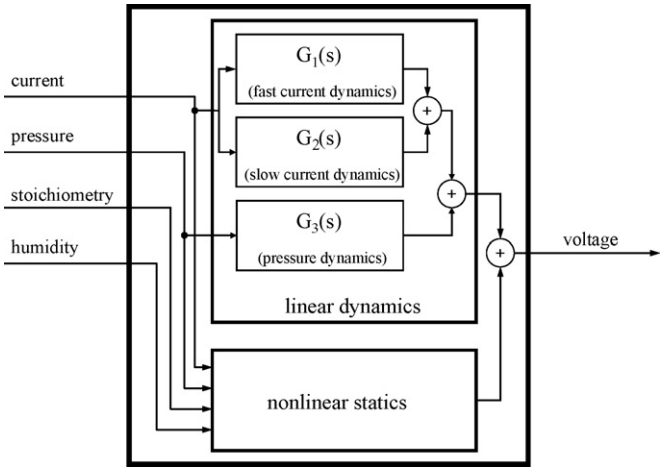

Fig. 3. Structure of the developed model.

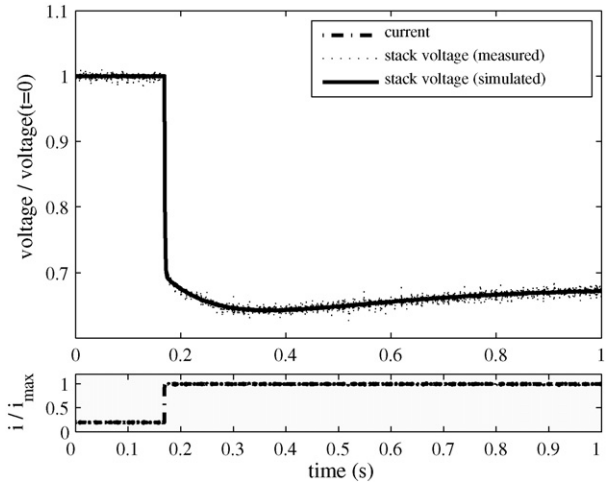

Fig. 4. Measured and identified voltage response to a high current density step.

3.3. Linear dynamic subsystem

In Ref. [15] some current steps are investigated. The time constant of the voltage response is in the range of 50–150 ms. Additionally in Ref. [16] a slow process (10–100 s) after current steps can be seen. Both observations together suggest a parallel structure for current dynamics, one for the slow and another for the fast process.

In Ref. [1] an RC-element models the fast current dynamics in a first approximation but is not precise enough. In Ref. [17] there can be seen some voltage overshooting at negative current steps and some undershooting at positive current steps, respectively. A description for this effect is given in Ref. [19].

Modelling the transient behaviour in DMFC with transfer functions was applied in Ref. [18]. Translated to process models a RC-element equals a PT1-element with the transfer function:

$$G_{\mathrm{PT1}}(s) = \frac{K_1}{(T_1 \cdot s + 1)}. \tag{1}$$

As mentioned just with a PT1-element the model fit on fast current dynamics is not good enough. In some cases the measured stack voltage shows a light over- or undershooting (see Fig. 4). To improve the model quality parallel a PT2Z-element, with the transfer function:

$$G_{\mathrm{PT2Z}}(s) = \frac{K_2(T_z \cdot s + 1)}{(T_2 \cdot s + 1) \cdot (T_3 \cdot s + 1)} \tag{2}$$

was added.

The slow current dynamics are quite different to the fast current dynamics. Here a massive overshoot in case of load reduction and an undershoot of stack voltage at positive current steps can clearly be seen (see Fig. 7). In the first few seconds after a load step a rapid decrease of over- and undershooting can be seen. After that initial approach stack voltage comes slowly closer to steady-state conditions. Therefore, the slow current dynamics were built with three basic elements. Two parallel differential elements, so-called DT1-elements, were connected with a static gain element (P-element) in series.

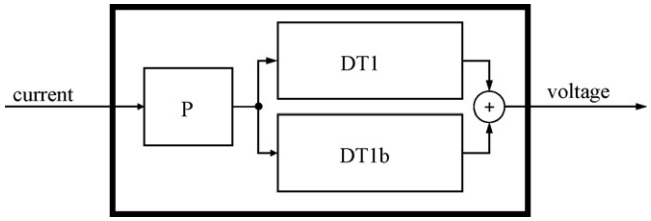

Fig. 5. Internal structure of the slow current dynamics element.

The transfer functions of these three elements are:

$$G_{\mathrm{DT1a}}(s) = \frac{T_4 \cdot s}{(T_4 \cdot s + 1)}, \tag{3}$$

$$G_{\mathrm{DT1b}}(s) = \frac{T_5 \cdot s}{(T_5 \cdot s + 1)}, \tag{4}$$

$$G_{\mathrm{P}}(s) = K_3. \tag{5}$$

Fig. 5 gives a look inside the slow current dynamics block.

For the cathode pressure dynamics the same structure as for the slow current dynamics was used, because once again over- or undershooting of steady-state stack voltage together with a faster and a slower approach can be seen.

In some preliminary investigations gas humidity and cathode stoichiometry do not show fast dynamic behaviour in the investigated operating area.

4. Simulation results

The dynamic input signal for each simulation was the measured current density or cathode pressure signal, respectively. All other model inputs were kept constant.

4.1. Fast current dynamics

The shape of voltage response within the first second after a load step depends on the operating point, the applied amplitude of the step and the direction of the step.

This reliance prevents the use of fixed model parameters for simulating varied conditions. This problem was solved by identifying the five current density levels one parameter set for each of the eight different load steps in the centre of the operating area.

These 40 records of model parameters were stored in a look-up-table. For simulating the fast dynamics of a load steps with the amplitude A at a current density B the matching parameter set was read from the look-up-table and used for all simulations with these AB conditions. If pressure, stoichiometry and humidity exactly match the identified case, simulation results fit precisely the measured data. If these parameters differ, a certain difference between simulation and measured data occurs. Both scenarios are shown in Fig. 6.

4.2. Slow current dynamics

For simulations a fixed set of model parameters was used for the slow current subsystem. The results for four positive and

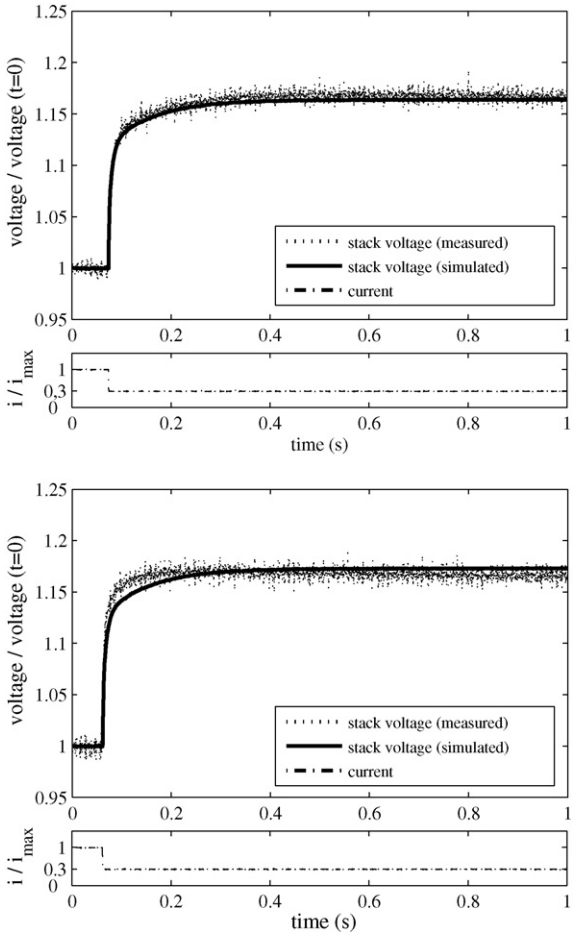

Fig. 6. Comparison of measured and simulated stack voltage in case of fast current dynamics (top: all input parameters are the same like in the case used for identification, bottom: measured data are at a lower pressure and stoichiometric level).

four negative load steps are shown in Fig. 7. The model shows in the centre of the investigated operating area a good agreement between simulated and measured fuel cell stack voltage. At the edges of the operating area the chosen model parameters do not

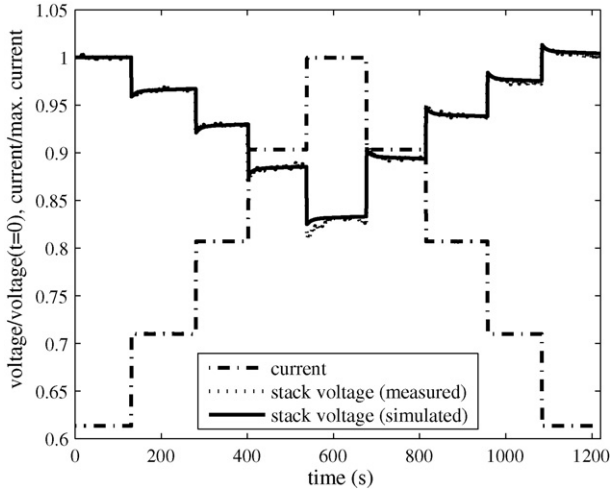

Fig. 7. Comparison of measured and simulated stack voltage in case of slow current dynamics.

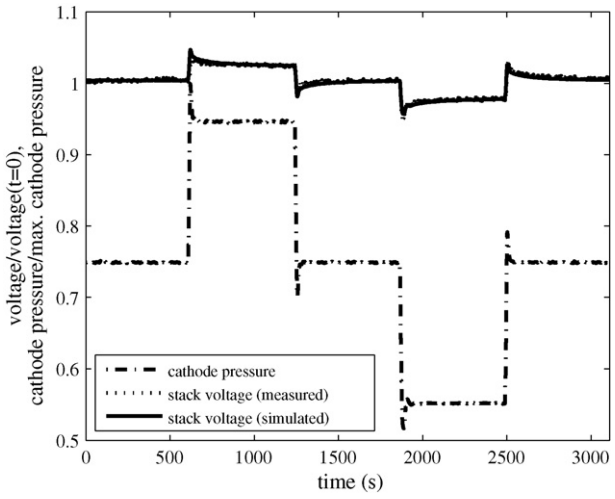

Fig. 8. Comparison of measured and simulated stack voltage in case of pressure dynamics.

match the measured voltage well. In Fig. 7 this can easily be seen at time range between 500 and 700 s. Here the highest possible current density was applied and the stack voltage drops deeper than the model predicts. This failure often can be observed at high current densities.

4.3. Cathode pressure dynamics

To model the cathode pressure dynamics the same model structure as for the slow current dynamics was used. And for the pressure model a fixed set of model parameters was used for simulations. In Fig. 8 the results of four pressure steps can be seen.

The peak in the pressure line after a step are caused by the test bench, especially by the setup of the controller parameters of the pressure valves. Due to the low sampling rate (1 Hz) of this measurement the really occurred height of the pressure peaks could be higher than the plotted one. This should be taken into account when the quality of the simulation results is judged. Once again in the centre of the investigated operating area the model fits measured data well apart from the very first moments after the step where the goodness is a bit lower. At the edges of the investigated area the fit loses accuracy.

4.4. Simulation time

It took less than 40 s to simulate 100 times a step with a length of 1000 ms at a sampling rate of 5000 Hz. This results in a total computing time of less than 1 ms per single step and fulfils the requirement.

5. Conclusion

With the developed Uryson-Model a modern PEM fuel cell stack can be modelled precisely. It is shown that the transient behaviour within the first second after current density

step can be simulated by a parallel PT1–PT2Z-element. Operation point depending model parameters improve the model quality in a wide operating area. It is also shown that a parallel combination of two DT1-elements in series with a P-element both the slow current dynamics as well as the pressure dynamics can be modelled. Without any optimisations in model code or programming work the developed model computes dynamic behaviour of a fuel cell stack faster than real-time, so the shown process model approach meets this requirement.

6. Future work

To improve model quality especially at the outer points of the operating area in future a mathematical description for the dependency of model parameters to the actual operating point will be focused. Further dynamic input parameters like humidity and excess ratio must be added as well as an expansion of operating area to reach readiness for automotive applications. A reduction of experimental effort should be reached by some statistically DOE or an artificial neuronal network approach.

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