

Modelling PEM Fuel Cell Stacks for FDI Using Linear Subspace Identification

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Abstract—A long life time and safe operation are important issues when polymer electrolyte membrane fuel cell (PEMFC) stacks are used as power supply in technical systems. Therefore, methods are needed to detect deviations from the chosen operating point before any damage to the stack or the environment occurs. In applications like vehicles, the fuel cell operation is highly dynamic, and special diagnosis cycles can not be used during operation. Thus, a diagnosis system is needed which uses the high dynamic data from operation. However, due to limitations of computational power, this diagnosis system must be as simple as possible.

In this paper, the linear canonical variate analysis (CVA), which is a subspace identification method, is used as a means for modelling the non-linear PEMFC stack. The linear state-space models can be shown to represent well the input-output behavior of the stack. Additionally, two concepts are proposed using state-space models from linear CVA for diagnosis purposes.

Index Terms—Fault Detection/Accommodation, Identification, Automotive Applications, Canonical Variate Analysis, Kalman Filter

I. INTRODUCTION

Polymer electrolyte membrane fuel cells (PEMFCs, also called proton exchange membrane fuel cells) are still subject to today's research. Technical systems using these fuel cells as a source of electric power are in development as well. Several prototypes of such systems, e.g. vehicles, mobile applications, and stationary systems like power and heat supply in residential houses, are already in operation.

For the commercialisation, a long life time and safe operation of PEMFC stacks are objectives that need to be achieved. For both, it has to be made sure that the actual operating point conforms with the operating point chosen by the controller. If the operating point is outside the nominal operating range, the degradation of the PEMFCs can be much higher than within and thus reduce the life time of the stack significantly. Therefore, such deviations have to be detected early and their causes have to be identified, i.e. a fault detection and isolation (FDI) method for such PEMFC stacks is needed. Performing the FDI task on-line allows the control system of the PEMFC stack to react fast in an appropriate manner and therefore reduce the risk of degradation or system failures. For the development of such control strategies and on-line diagnosis tools, computationally fast and accurate dynamic models of the PEMFC stack are required.

In literature, diagnosis methods for PEMFCs are often presented for only one fault, e.g. liquid water in the electrodes [1], [2]. Others build on special measurement methods like impedance spectroscopy (e.g. [3]). Only very few papers have been published on on-line diagnosis methods for PEMFC stacks, e.g. [4], [5], [6]. In [4], [5], the stack output voltage is predicted using a model and is then compared to the measured stack voltage for diagnosis. [6] is developed for stationary applications and based on current-voltage characteristics, also called polarisation curves, which are described by a parametric model. Fuzzy clusters of parameter deviations are then used for FDI.

This paper focuses on the modelling aspect for on-line diagnosis methods for PEMFC stacks in highly dynamic operation modes, which can be found in fuel cell powered vehicles, for example. In this case, the model has to comprise the dynamic response of the stack on changes in one or more of the various inputs without being computationally expensive for not loosing the model-based on-line diagnosis capability. Additionally, the diagnosis result must be acquired from normal operation data, because special diagnosis cycles, like current-voltage characteristics in [6], can not be measured during dynamic operation.

In literature, many modelling approaches are based on the description of the physical and chemical processes in a fuel cell stack, either as systems of (partial) differential equations or as electrical circuits, e.g. [7], [8]. These models are often very detailed, but they comprise many unknown parameters which are difficult to identify. Also, if all possible inputs of the system should be considered, these models are not suitable for an required on-line implementation on microcontrollers.

Recently, dynamic modelling approaches have been published considering several input signals, e.g. [9], [10]. These approaches are empirical and comprise system identification from dynamic measurements, resulting in rather simple and computationally fast models. They represent the input-output behaviour of the stack well, but do not provide information on internal signal values like humidity of the membrane etc. These input-output behaviour models are often sufficient to design the controller or FDI system. Therefore, this approach is also used in this contribution.

Drawbacks of the approaches [9], [10] are the required high number of measurements in steady state and the com-

putational expensive non-linear optimisation of the model parameters. Additionally, in [9] cross-influence on the dynamics for changes in different input signals are not accounted for. Here, these drawbacks are reduced by using a linear state-space model retrieved from canonical variate analysis (CVA), a so-called subspace identification method. It will be shown that such a linear state-space model can reproduce the dynamic behaviour of a PEMFC stack well with relatively small system orders.

Based on such state-space models, two diagnosis approaches will be outlined and first results will be presented. All results were developed with measurement data provided by an industry partner.

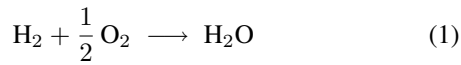
The paper is structured as follows: Section II describes the functionality of a PEMFC stack and stack measurements used in this work. The idea of CVA as one type of subspace identification methods is outlined in Section III. Simulation results using a state-space model gained by CVA are presented in Section IV. In Section V, two diagnosis concepts using a CVA state-space model are outlined and first results are presented. The paper closes with a conclusion in section VI.

II. THE PEMFC STACK

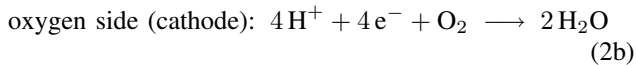
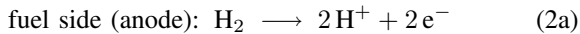
The first part of this section provides a short overview of the functionality of a PEMFC stack in general (for further information, refer e.g. to [11]). Information on the specific stack used for the measurements and a description of the measurement data used for this work are given in the second part of this section.

A. Functionality of a PEMFC Stack

In fuel cells, chemical energy stored in the fuel is transformed directly to electric power with high efficiency. For PEMFCs, hydrogen is used as fuel and pure oxygen or air is used as oxidant. The exhaust comprises of water and the remaining parts of the gases which did not take part in the reactions. Overall, the chemical reaction



is the same like for the combustion of the fuel, but it is separated into two half-cell electrochemical reactions:



These two reactions are separated by a special membrane, which conducts only hydrogen ions (protons), but not electrons. The scheme of one PEM fuel cell is depicted in Fig. 1.

For a good proton conductivity, the membrane has to be humidified. This happens automatically by the product water and can be influenced additionally by humidification of the supplied gases. The pressure and the flow rate of the supplied gases can normally be adjusted by valves mounted at the inlets and outlets of the stack. In this paper, pressure means the over pressure compared to ambient pressure. The

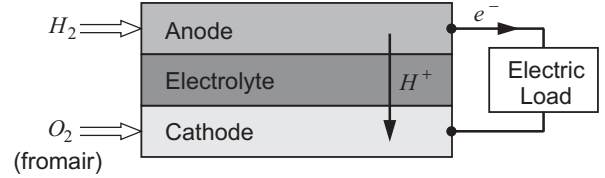


Fig. 1. Scheme of a single PEM fuel cell

pressure difference between the anode and the cathode has to be small enough so that the membrane is not damaged (normally below 0.5 bar).

Operating temperatures for PEMFCs vary between 30 °C and 100 °C, although PEMFCs for higher and lower temperature ranges are also in development. The chemical reaction in fuel cells is an exothermal reaction, i.e. heat is a by-product. For the thermal management, a cooling or heating/cooling system is necessary, which is normally realized by an air flow or water flow, respectively, in separated flow channels in the cells. Water can be used to heat up the stack for start-up as well. If water is used, the (medial) stack temperature is often assumed to be equal to the temperature of the water at the outlet of the stack.

Depending on the electric current, each single PEMFC is normally operated at a voltage between approximately 0.4 V and 1 V (see e.g. [11] for a more detailed explanation of the cell potentials). In addition to the operating parameters like gas supplies etc., the possible current depends also on the cell area. Therefore, the current density is often used as the regarded input signal instead. A fuel cell stack is a serial connection of several single fuel cells.

A fuel cell stack can be operated either in galvanostatic or potentiostatic mode. In galvanostatic mode, which will be used in the following, the current is imposed on the stack. For this current, the stack provides a specific voltage depending on the operating conditions (operating mode). In potentiostatic mode, the stack voltage is imposed on the stack.

The consumptions of fuel and oxidant depend on the electric current flowing through the cell. The ratio between provided fuel (oxidant) and consumed fuel (oxidant) is called fuel (oxidant) stoichiometry λ_{H_2} (λ_{O_2}). The stoichiometries are often used as input values instead of the corresponding gas flows. Please note that although air is used as cathode gas, the corresponding stoichiometry is denoted by λ_{O_2} , because oxygen is the only air component taking part in the reaction. Using air as oxidant means that the gas flow at the cathode side has to be five times higher compared to using pure oxygen due to the fact that the air consist of only about 20% oxygen.

Fuel cell systems can be built with an anode recycling loop for a better fuel utilisation, i.e. the anode exhaust is fed in again as anode input gas. Doing so, the anode gas enriches with diffusing nitrogen from the cathode side. Because test systems often have no anode recycling loop, the effect is simulated by using a gas mixture of hydrogen and nitrogen instead of pure hydrogen as anode gas. The percentage of

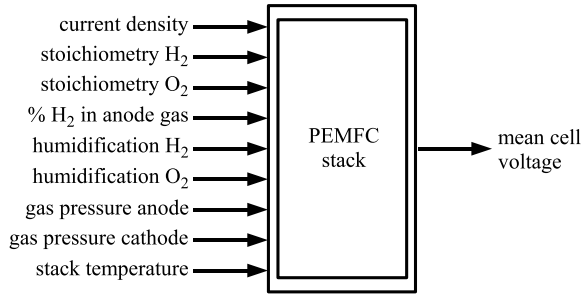


Fig. 2. System theoretical scheme of a PEMFC stack

hydrogen in the anode gas is therefore another input signal of the stack.

From the system theory's point of view, a PEMFC is a dynamic, non-linear multiple input, single output (MISO) system (cf. Fig. 2). The inputs are the imposed current density, the gas pressures, the stoichiometries of the reactants, and the heating/cooling temperature (or stack temperature). The output of the system is the mean cell voltage of the stack.

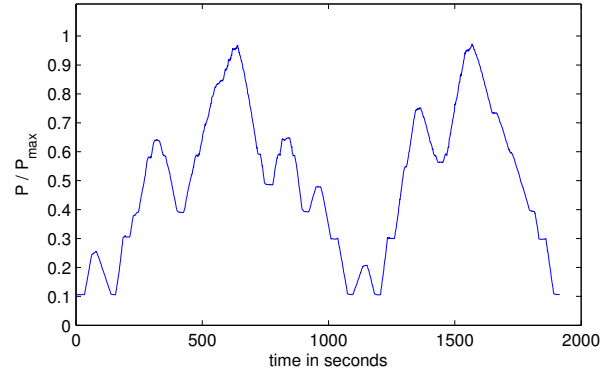
B. PEMFC Stack Measurements

With regard to the designated application in vehicles, the two load profiles shown in Fig. 3 were chosen similar to existing driving cycles. An existing standardized driving cycle like the new European driving cycle (NEDC) could not be realized due to test bench limitations.

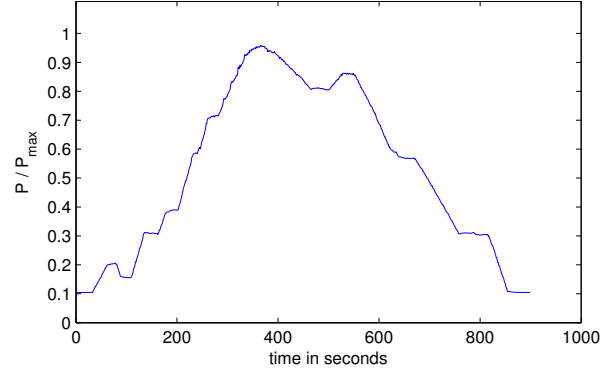
The PEMFC stack measurements have been carried out by an industry partner using a proprietary stack with 20 cells. For the development of FDI methods, the nine input signals shown in Fig. 2 have been varied and recorded together with the mean cell voltage with a rate of 1 Hz. All input signals were chosen in the normal operation mode as functions of the imposed current density.

The five input signals given in Table I will not be measurable in an operational PEMFC system. For each of them, deviations from the normal operating conditions were investigated as the failure modes to detect. Each failure mode was imposed on the stack by increasing or decreasing the nominal values from 100% to the desired percentage during one load cycle. Then the failure mode was held for one cycle and afterwards either brought back to 100% or to the next failure mode of the same input within one load cycle. All failure modes have been regarded solely except for the humidifications. For these two input signals, all combinations of failure modes have been investigated.

The measurement procedure of these various load cycles accumulates to a identification data set of more than 335.000 data points (over 93 h) and a validation data set of more than 155.000 data points (over 43 h). For the five inputs with failure modes, the variation ranges including failure mode operation are also given in Table I. For the other inputs, the ranges are as follows: current density $\Delta j = 1.1 \text{ A/cm}^2$, gas pressures $\Delta p_{H_2} = \Delta p_{O_2} = 1.4 \text{ bar}$, stack temperature $\Delta \vartheta_{\text{Stack}} 22 \text{ K}$.



(a) Load cycle for identification



(b) Load cycle for validation

Fig. 3. Load cycles used for PEMFC stack measurements

III. CANONICAL VARIATE ANALYSIS (CVA)

The CVA is a subspace identification method and was first introduced by Larimore in [12]. A good overview of the CVA methodology is given in [13]. A review of subspace identification algorithms was done recently in [14], whereas the focus lays on the three best known algorithms, namely “numerical algorithms for subspace state-space system identification (N4SID)”, “multivariable output error state-space identification (MOESP)”, and CVA.

The main idea behind these subspace identification methods is to reconstruct the Kalman filter state sequence directly from measured input/output data of the system. With this state sequence, the state matrices are estimated optimally in a least squares sense. Due to additive noise on the input/output observations of the system, in general, the estimated state order is the maximum order possible for the available number of observations. Therefore, the subspace algorithms divide this high order state space into a signal subspace and a noise subspace by using a (generalized) singular value decomposition (SVD). The (low order) signal subspace equals the estimated system state space, the noise subspace is neglected. In other words, the system order is part of the identification result and not an assumption in the beginning of the identification process. In general, the states of a subspace identification model do not have any physical meaning.

The two algorithms N4SID and MOESP have been developed using geometrical considerations, CVA is based on

TABLE I
FAILURE MODES FOR NON-MEASURABLE INPUTS

| input | range | Failure mode in % of the nominal operating value | | | | |
|-------------------------------|------------------------------|--|-----------|-------------|-------------|-------------|
| | | upwards 1 | upwards 2 | downwards 1 | downwards 2 | downwards 3 |
| % H ₂ in anode gas | $\Delta rate_{H_2} = 61\%$ | 125 | - | 75 | 50 | - |
| Stoichiometry H ₂ | $\Delta \lambda_{H_2} = 3.4$ | 144 | - | 94 | 85 | - |
| Stoichiometry O ₂ | $\Delta \lambda_{O_2} = 3.0$ | 182 | - | 94 | 85 | - |
| Humidification H ₂ | $\Delta rh_{H_2} = 269\%$ | 200 | - | 40 | - | - |
| Humidification O ₂ | $\Delta rh_{O_2} = 225\%$ | 214 | 286 | 86 | 57 | 43 |

multivariate statistical analysis. In [15], it was shown that all three algorithms can be described by a generic algorithm based on the geometrical derivation. They only differ in weighting matrices. Based on this unifying theorem, e.g. [16], [17], [18] as well as the survey [14] give a good introduction to subspace identification. An implementation of N4SID and CVA based on such a geometrical algorithm is available in the SYSTEM IDENTIFICATION TOOLBOX in MATLAB [19].

In the comparison of subspace identification algorithms, besides other advantages, it was shown that CVA is close to the maximum likelihood (ML) solution and the numerical stability of its original implementation based on regression is better than of geometrical algorithms [20]. With the ADAPT_X software [21], a multivariate statistic based implementation of the CVA algorithm is also commercially available as a MATLAB extension.

The CVA for linear time-invariant (LTI) systems is based on a discrete-time state-space description of the system under investigation given by

$$\mathbf{x}_{k+1} = \mathbf{A} \mathbf{x}_k + \mathbf{B} \mathbf{u}_k + \mathbf{w}_k \quad (3a)$$

$$\mathbf{y}_k = \mathbf{C} \mathbf{x}_k + \mathbf{D} \mathbf{u}_k + \mathbf{G} \mathbf{w}_k + \mathbf{v}_k, \quad (3b)$$

whereas $\mathbf{x}_k \in \mathbb{R}^n$ is the state vector, $\mathbf{u}_k \in \mathbb{R}^p$ is the input vector and $\mathbf{y}_k \in \mathbb{R}^q$ is the output vector, each at the time $t = k T_s$ and with the sample time T_s . The length n of the state vector is the order of the system. The the vectors $\mathbf{w}_k \in \mathbb{R}^n$ and $\mathbf{v}_k \in \mathbb{R}^q$ are process noise and measurement noise, respectively.

Starting from measurement data of the inputs and outputs, estimates of the unknown order n of the system and the unknown system matrices \mathbf{A} , \mathbf{B} , \mathbf{C} and \mathbf{D} as well as estimates of the covariance matrices of the noise processes are calculated by the CVA algorithm. One can choose if a model with or without the direct coupling matrix \mathbf{D} should be estimated by the algorithm.

IV. SIMULATION MODELS

Using ADAPT_X CVA for modelling fuel cells was already proposed in [22] for a single input, single output (SISO) model of a direct methanol fuel cell (DMFC), where only the current density is used as input signal. In [10], a geometric algorithm with CVA weighting is used to model the linear dynamic part of a Uryson model structure, a parallel connexion between a non-linear static part and a linear dynamic

TABLE II
MODEL ORDER AND STATISTICAL DATA FOR THE SIMULATION
RESULTS FOR NORMALISED OUTPUTS $U_{cell} / U_{cell,max}$

| Model | Order | Identification data set | | validation data set | |
|--------------------|-------|-------------------------|----------------------|---------------------|----------------------|
| | | Mean | St.Dev. | Mean | St.Dev. |
| w/out \mathbf{D} | 9 | $0.3 \cdot 10^{-3}$ | $18.4 \cdot 10^{-3}$ | $4.3 \cdot 10^{-3}$ | $18.6 \cdot 10^{-3}$ |
| with \mathbf{D} | 10 | $0.5 \cdot 10^{-3}$ | $19.4 \cdot 10^{-3}$ | $7.9 \cdot 10^{-3}$ | $19.1 \cdot 10^{-3}$ |

part, for a PEMFC. There, only the current density and the oxygen stoichiometry are inputs to the dynamic part.

In this paper, the ADAPT_X implementation of the linear CVA is applied to model the PEMFC stack on the whole, using all nine input signals as inputs to the model. For the approximation of the non-linear behaviour of the PEMFC stack by a linear state-space description, models with and without direct coupling matrix have been investigated.

The models were estimated with the identification data set and used for simulation for both data sets. The mean and standard deviation (St.Dev.) for the simulation results and the orders of the models can be found in Table II. One can see that both approaches deliver a good simulation model with an almost vanishing mean and small standard deviations for both data sets. The model without direct coupling matrix \mathbf{D} performs better with a smaller model order.

By replacing the output equation (3b) with the equation

$$\mathbf{y}_k = \mathbf{C} \mathbf{x}_k + \mathbf{D} \mathbf{u}_k - \mathbf{y}_B + \mathbf{G} \mathbf{w}_k + \mathbf{v}_k, \quad (4)$$

with an additional bias $-\mathbf{y}_B$, the simulation results have zero mean for the identification data set and almost zero mean for the validation data set without changing the standard deviations.

In Fig. 4, the mean cell voltage simulation for the model of order 9 without direct coupling matrix \mathbf{D} and bias as well as the respective voltage measurement are plotted for one normal operation cycle of the validation data set. These results show that the non-linear PEMFC behaviour can be approximated well by a linear state-space model with a relatively small order.

V. PEMFC DIAGNOSIS CONCEPTS BASED ON CVA STATE-SPACE MODELS

In this section, two diagnosis concepts are introduced which are based on state-space models from CVA identification. Both approaches estimate the unknown inputs, FDI can then easily be done using thresholds for the estimated signals.

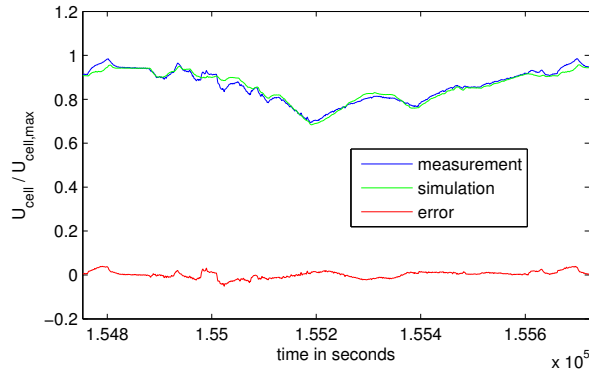


Fig. 4. Simulated (model without D , order 9) and measured mean cell voltage of one normal operation cycle from the validation data set

So far, the oxygen stoichiometry failure modes have been studied with both concepts using state-space-models without direct coupling matrix D . The first part of this section describes the usage of a Kalman Filter for the estimation task. An inverse model approach is described in the second part of this section.

A. Kalman Filter

This diagnosis concept is based on a state-space model like the presented simulation models:

$$\mathbf{x}_{k+1} = \mathbf{A}\mathbf{x}_k + \begin{bmatrix} \mathbf{B}_1 & \mathbf{B}_2 \end{bmatrix} \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{bmatrix}_k + \mathbf{w}_k \quad (5a)$$

$$\mathbf{y}_k = \mathbf{C}\mathbf{x}_k + \begin{bmatrix} \mathbf{D}_1 & \mathbf{D}_2 \end{bmatrix} \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{bmatrix}_k + \mathbf{v}_k, \quad (5b)$$

whereas \mathbf{u}_1 are the measurable inputs and \mathbf{u}_2 are the non-measurable inputs. As in Section IV, it is assumed that all inputs can be measured for the identification process.

To use this model in a Kalman filter to estimate the non-measurable inputs, these inputs are assumed to be constant states of the system:

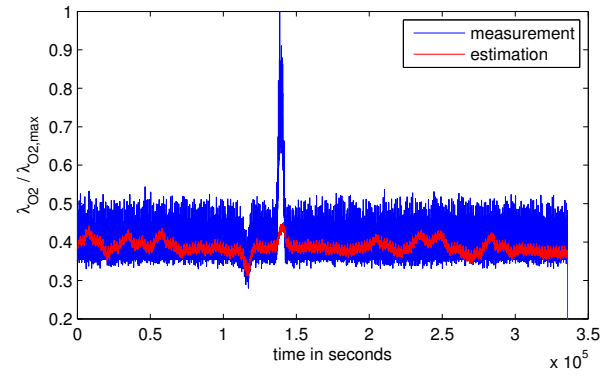
$$\begin{bmatrix} \mathbf{x} \\ \mathbf{u}_2 \end{bmatrix}_{k+1} = \begin{bmatrix} \mathbf{A} & \mathbf{B}_2 \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{u}_2 \end{bmatrix}_k + \begin{bmatrix} \mathbf{B}_1 \\ \mathbf{0} \end{bmatrix} \mathbf{u}_1 + \tilde{\mathbf{w}}_k \quad (6a)$$

$$\mathbf{y}_k = \begin{bmatrix} \mathbf{C} & \mathbf{D}_2 \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{u}_2 \end{bmatrix}_k + \begin{bmatrix} \mathbf{D}_1 \\ \mathbf{0} \end{bmatrix} \mathbf{u}_1 + \mathbf{v}_k. \quad (6b)$$

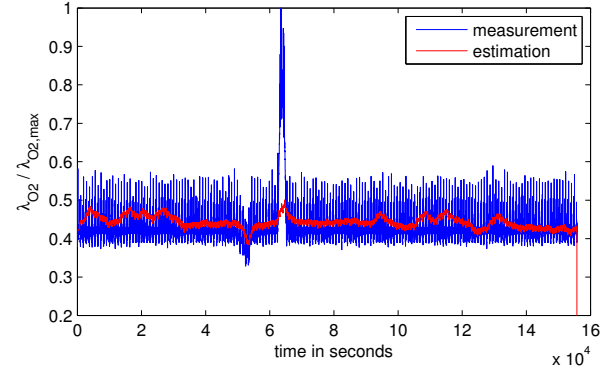
Now, the extended state vector can be estimated by using a Kalman filter. For this work, a modified Kalman filter was implemented, where the covariance between the state and the system noise is estimated in each filter step additionally.

From the measurement data of the PEMFC stack, only the measurable inputs and the oxygen stoichiometry have been used for identifying a model for the Kalman filter with the ADAPT_X CVA algorithm. The observation results of the Kalman filter for this model of order 17 are shown in Fig. 5. Note that the whole data sets with changes in all inputs are shown.

One can see that the Kalman filter estimates the mean value well, but does not follow the variations within one



(a) Results for the identification data set



(b) Results for the validation data set

Fig. 5. Kalman filter estimates of the oxygen stoichiometry

cycle. For failure modes with a lower oxygen stoichiometry than normal, the Kalman filter estimate follows the mean value of the cycles well. The failure modes with an upward deviation are not followed that good, and the deviations in the other parts of the data sets can not be distinguished from this case.

From this, it can be concluded that the Kalman filter approach can be used to diagnose reductions of the oxygen stoichiometry. It delivers estimates of a low-pass filtered value of the oxygen stoichiometry, but the performance for upward deviations is not yet satisfying. Further research will be done to improve these results, e.g. by using non-linear transformation of the inputs for a higher sensitivity of the model.

B. Inverse Model

For this diagnosis concept, the CVA algorithm is used to retrieve a model which uses all measurable stack inputs and the mean cell voltage as additional input and calculates the non-measurable stack inputs. This concept is depicted in Fig. 6. The results for the estimation of the oxygen stoichiometry using such an inverse model are shown in Fig. 7. The model order is 14.

Like with the Kalman filter, the oxygen stoichiometry estimates of this approach do not follow the variations within one cycle, but stay close to the mean value. For the failure mode with lower oxygen stoichiometries, the mean value is followed well. For the failure modes with

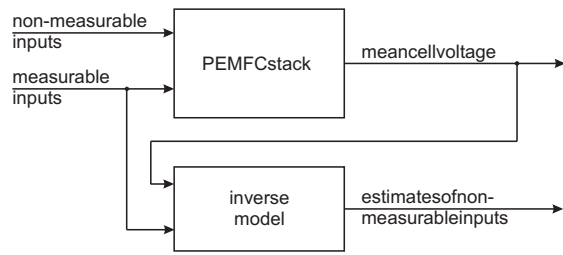


Fig. 6. Inverse model concept for diagnosis

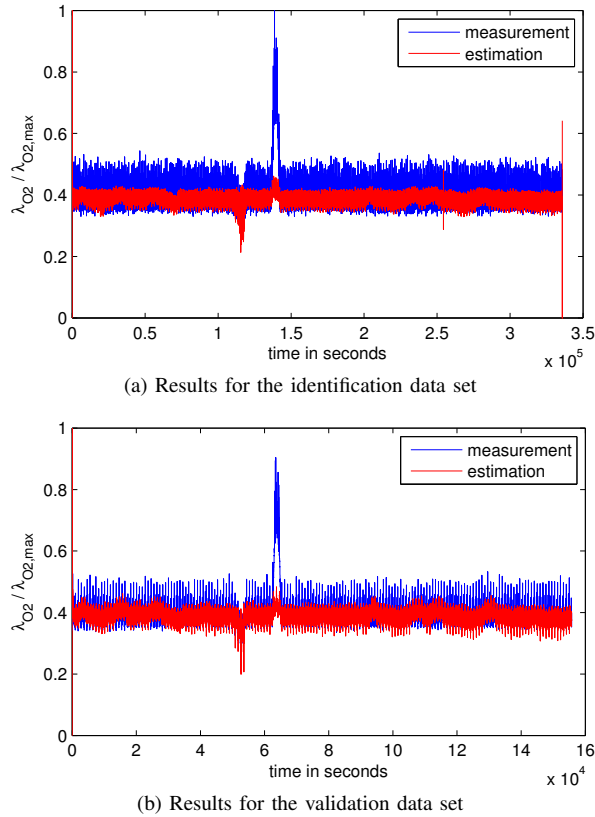


Fig. 7. Inverse model estimates of the oxygen stoichiometry

a higher oxygen stoichiometry than normal, the values are underestimated. In contrast to the Kalman filter approach, both failure modes can be diagnosed. If this approach should be used for the observation of the mean value, an appropriate exponential weighting of the inverse model output could be chosen to reduce the underestimation of the higher oxygen stoichiometry values.

VI. CONCLUSIONS

In this paper, it was shown that linear CVA state-space models with a relatively low order are able to represent the non-linear behaviour of a PEMFC stack well in the regarded operating range for load cycles similar to driving cycles of vehicles. Additionally, two concepts, a Kalman filter and an inverse model, were introduced which show how CVA state-space models can be used for diagnosis of non-measurable inputs. Both concepts were so far studied for the oxygen stoichiometry. The Kalman filter has been shown to work

as FDI for lower values than normal, the inverse model approach showed good diagnosis results for all failure modes of the oxygen stoichiometry.

Further research will comprise the investigation of the other non-measurable inputs. Additionally, the non-linear extension of the CVA will be tested to improve the diagnosis results.

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