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Nonlinear data-driven identification of polymer electrolyte membrane fuel cells for diagnostic purposes: A Volterra series approach

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HIGHLIGHTS

- Broad-band excitation signals are used for nonlinear model identification.
- A frequency domain description is obtained by the harmonic probing algorithm.
- The electrochemical impedance is equivalent to the first order Volterra kernel.
- Nonlinear output responses are described by higher order Volterra kernels.
- Proper excitation signals for fault detection are obtained through optimization.

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ABSTRACT

In this work, a data-driven identification method, based on polynomial nonlinear autoregressive models with exogenous inputs (NARX) and the Volterra series, is proposed to describe the dynamic and nonlinear voltage and current characteristics of polymer electrolyte membrane fuel cells (PEMFCs). The structure selection and parameter estimation of the NARX model is performed on broad-band voltage/current data. By transforming the time-domain NARX model into a Volterra series representation using the harmonic probing algorithm, a frequency-domain description of the linear and nonlinear dynamics is obtained. With the Volterra kernels corresponding to different operating conditions, information from existing diagnostic tools in the frequency domain such as electrochemical impedance spectroscopy (EIS) and total harmonic distortion analysis (THDA) are effectively combined. Additionally, the time-domain NARX model can be utilized for fault detection by evaluating the difference between measured and simulated output. To increase the fault detectability, an optimization problem is introduced which maximizes this output residual to obtain proper excitation frequencies. As a possible extension it is shown, that by optimizing the periodic signal shape itself that the fault detectability is further increased.

1. Introduction

To ensure safe operation, prolonging the life-time and avoiding critical failure of proton exchange membrane fuel cells (PEMFCs), reliable on-line diagnosis methods are desired. Existing techniques can be loosely categorized into being model-based as in Refs. [1–3], or non-parametric methods based on polarization curve or electrochemical impedance spectroscopy (EIS) measurements [4–6]. Whereas the polarization curve describes the static relation between current and voltage, EIS makes use of a superimposed AC signal either in galvanostatic or potentiostatic mode with a certain frequency and a reasonable small amplitude, in order for the system response to be primarily linear. The gain and phase of the system response are estimated. Repeated for a wide range of excitation frequencies (e.g 0.1 Hz - 20 kHz [7]) the electrochemical impedance of the fuel cell, which can be thought of as the linear transfer function, is characterized. System faults are then being detected as a change of the electrochemical impedance. Carrying out a complete EIS takes a significant amount of time and may not be suitable for fast detection of system faults. To reduced the necessary experimental time, broad-band excitation signals have been utilized such as multi-harmonic excitation signals [8–10] or pseudo-random binary sequence perturberation [11]. For the on-line diagnosis it is advantageous to continuously monitor the impedance at a single frequency of interest, such as in the high frequency resistance method [12,13]. Although good results in

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system diagnosis of PEMFCs have been obtained by EIS, it is sometimes difficult to differentiate certain system faults such as flooding and CO-poisoning under certain operating conditions [14]. Therefore, research interest has turned towards analyzing nonlinear effects in recent years such as total harmonic distortion analysis (THDA) [15–18]. Thereby, the amplitude of the superimposed AC signal is increased in order to generate nonlinear system responses at the output (e.g. harmonics). The proper choice of the excitation signal is important to the task of detecting and discriminating system faults, and a multi-tonal excitation may be used to increase the available information for the on-line diagnosis. A more analytic approach of describing the fuel cell's nonlinear behavior by the means of the Volterra series was introduced in Ref. [19]. Therein, the issue of similar electrochemical impedance spectra for different system faults was addressed and fault discrimination was achieved by additionally considering the nonlinear system response. This has been done by experimentally estimating the Volterra kernels in the frequency domain. Due to its polynomial and non-parametric nature, the Volterra series inherently suffers from the curse-of-dimensionality and an estimation of the complete series is in general not possible. This aggravating fact was avoided by estimating only a subspace of the Volterra kernel, namely only those parts which correspond to a single harmonic excitation. The experimental setup is therefore similar to EIS and the procedure is repeated for a wide range of excitation frequencies. A multi-tonal excitation during on-line diagnosis would lead to additional nonlinear effects such as the generation of signal content at intermodulated frequencies which are not captured by the Volterra kernel subspace estimation.

In this work, a polynomial nonlinear autoregressive model with exogenous inputs (NARX) in the time domain [20] is identified using a broad-band excitation signal, effectively decreasing the necessary experimental time. This model is then transformed into a Volterra series representation in the frequency domain via the harmonic probing algorithm [21], thus obtaining the Volterra kernels up to a predefined order. Identifying the Volterra kernels for nominal and faulty system states and analyzing their differences provides a comprehensive framework for describing linear and nonlinear output responses, e.g. EIS and THDA, with respect to multi-harmonic excitations. Additionally, a time-domain optimization approach is presented, utilizing the NARX models for nominal and faulty operating conditions, as to obtain proper harmonic excitations for output-residual based fault detection. As a possible extension of this time-domain approach, the signal shape itself is subjected to optimization. The proposed method is demonstrated on simulated fuel cell voltage/current data based on a simulation model presented in Ref. [22]. Thereby, the feedgas dynamics inside cathode, anode, inlet and outlet manifolds are described by 0D-volumes and a membrane hydration model is included. Additional auxiliary components such as the air compressor, a valve-controlled hydrogen tank and a humidifier are considered as well. Electrochemical processes are modeled by static relations based on the nernst equation and accounting for activation, polarization and concentration losses.

2. Methodology

In this section, the methodology and relevant fundamentals are discussed. At first the Volterra series, the corresponding nonlinear output responses and its relation to EIS and THDA are given. Thereafter the data-driven NARX model identification and the harmonic probing algorithm, as to obtain the Volterra kernels from the NARX models, are outlined. A short example is given as to facilitate the interpretation of higher order Volterra kernels. Lastly, it is shown how the NARX models for different operating conditions can be used as to obtain an optimal excitation signal to increase the detection of faults.

2.1. Volterra series

In nonlinear system identification, the Volterra series has been extensively studied as it provides an elegant way of describing nonlinear effects in time domain as well as in the frequency domain. Starting from the linear system description, the Volterra series will be explained to highlight the important properties which directly relate to the electrochemical impedance and the description of nonlinear harmonics. For a more detailed discussion on the Volterra series the reader is referred to [23].

It is well known, that the response $y(t)$ of a linear time-invariant system to an arbitrary input $u(t)$ is described by the convolution integral

$$y(t) = \int_0^\infty h(\tau)u(t-\tau)d\tau, \tag{1}$$

with $h(t)$ being the impulse response of the linear system. Investigating the system response for a harmonic input such as

$$u(t) = A\cos(\omega\, t) = \frac{A}{2}e^{i\omega t} + \frac{A}{2}e^{-i\omega t}, \tag{2}$$

leads to

$$y(t) = \frac{A}{2}e^{i\omega t}\underbrace{\int_0^\infty h(\tau)e^{-i\omega\tau}d\tau}_{H(\omega)} + \frac{A}{2}e^{-i\omega t}\underbrace{\int_0^\infty h(\tau)e^{i\omega\tau}d\tau}_{H(-\omega)}. \tag{3}$$

Since the terms on the right hand side are conjugate complex expressions, the equation above can be simplified as

$$y(t) = A\mathrm{Re}\left(e^{i\omega t}H(\omega)\right),$$

$$y(t) = A|H(\omega)|\cos(\omega\, t + \arg(H(\omega))), \tag{4}$$

with $H(\omega)$ being the Fourier transform of the impulse response describing the amplitude and phase of the output for a harmonic input with frequency ω and Amplitude A. Note, that for the fuel cell $H(\omega)$ is equivalent to the electrochemical impedance.

The Volterra series, capable of describing a wide range of nonlinear systems, can be seen as the polynomial extension of the linear convolution (1) and is given by

$$y(t) = \sum_{l=1}^{\infty}\int_0^\infty \dots \int_0^\infty h_l(\tau_1, \tau_2, \dots, \tau_l)\prod_{p=1}^{l} u(t-\tau_p)d\tau_p, \tag{5}$$

with $h_l(\tau_1, \tau_2, \dots, \tau_l)$ being the l-th order Volterra kernel. Note that the dimensionality of the kernel increases with the polynomial order. In practice, the infinite Volterra series is truncated at a certain order due to the diminishing contribution of higher order harmonics. Analogous to the linear case, the multi-dimensional Volterra kernel in the frequency domain is obtained by the multi-dimensional Fourier transformation

$$H_l(\omega_1, \dots, \omega_l) = \int_0^\infty \dots \int_0^\infty h_l(\tau_1, \dots, \tau_l)e^{-i(\omega_1\tau_1 + \dots + \omega_l\tau_l)}\prod_{p=1}^{l} d\tau_p. \tag{6}$$