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Online monitoring of state of charge and capacity loss for vanadium redox flow battery based on autoregressive exogenous modeling

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HIGHLIGHTS

- Autoregressive exogenous modeling with online adaption is proposed for VRB.
- A method for online SOC and capacity loss monitoring is proposed for VRB.
- H-infinity observer is used for state co-estimation.
- The proposed method is verified with lab-scale experiments.

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ABSTRACT

Accurate monitoring of state of charge (SOC) and capacity loss is critical for the management of vanadium redox flow battery (VRB) system. This paper proposes a novel autoregressive exogenous model for the vanadium redox flow battery, based on which the model-based monitoring of state of charge and capacity loss is investigated. The offline parameterization based on genetic algorithm and the online parameterization based on recursive least squares are investigated for the proposed model to compare the model accuracy and robustness. Leveraging the parameterized model, an H-infinity observer is exploited to estimate the battery state of charge and capacity in real time. Experimental results suggest that the proposed autoregressive exogenous model can accurately simulate the dynamic behavior of vanadium redox flow battery. Compared with the offline model based method, the observer based on online adaptive model is superior in terms of the accuracy of modeling, state of charge estimation and capacity loss monitoring. The proposed method is also verified with high robustness to the uncertain algorithmic initialization, electrolyte imbalance, and the change of system design and work conditions.

1. Introduction

Battery storage systems are at the forefront of applications in various fields such as renewables penetration, emergency back-up, smart grid and transportation electrification [1–3]. Among different battery chemistries, the all-vanadium redox flow battery (VRB) proposed by Skyllas-Kazacos and co-workers [4,5] has shown outstanding potential due to the unique features of cross contamination elimination, high energy efficiency, tolerance to deep discharge and long cycling life. Till now, lots of efforts have been made to improve the VRB performance, mostly in the field of new materials, electrolytes and design optimization [6,7]. However, some major challenges for the real application of VRB have not been adequately addressed.

The state of charge (SOC) which describes the percentage of remaining capacity to the total capacity is a key battery state to be monitored in a battery management system (BMS) [8]. Accurate SOC monitoring protects the VRB from rapid aging or damage caused by unsuitable over-charge and over-discharge. The coulomb counting (CC) method is a standard way to monitor the SOC of a broad range of battery chemistries. However, it requires a precise guess of the initial SOC and very accurate sensing without drift which are not typically met in real applications [9]. The VRB manifests itself by using additional

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open-circuit cells to directly measure the open circuit voltage (OCV) which is further used to infer the SOC. However, the additional open-circuit cells bring additional system complexities which are not favorable for the practical application. Methods involving the measurement of electrolyte properties have also been investigated. Skyllas-Kazacos et al. determined the SOC of the VRB by measuring the conductivity and spectrophotometric properties of the individual half-cell electrolytes [10]. Li et al. estimated the SOC of VRB by using the viscosity which was inferred from the measured pressure drop [11]. This method is insightful for online monitoring, although a range of other factors that can increase pressure drop could lead to erroneous measurements. Furthermore the system should be well designed with additional monitoring units.

The model-based SOC observers link the measured current and voltage to the immeasurable SOC via a nonlinear state-space model [12–16]. Due to the ease of adoption and reasonable accuracy, such methods appeal to real-time embedded systems provided that an highly accurate model is available [17]. Physics-based electrochemical models have been built to model the complicated dynamics in battery systems [18]. Several simplified mathematical models were proposed by Tang et al. by analyzing the key physical and chemical processes of VRB [19]. Such models are theoretically accurate but the key model parameters are mostly empirical depending on the extensive testing and the knowledge of battery dynamics. By comparison, the equivalent circuit models (ECMs) exhibit an excellent adaptability and a good balance between the accuracy and computing cost thus is a favorable template for online utilizations. Chahwan et al. [20] and Barote et al. [21,22] proposed a simple ECM consisting of a voltage source and a resistance to describe the dynamic behavior of VRB. However, the dynamic variability of a flow battery has been overlooked and the models also lack verification. Recently, ECMs with first order [23–25] or second order [26,27] RC networks were used to take the polarization effects of the VRB into account. Although the ECMs are practical in real-time embedded systems, they are constrained by the physical meanings of the electrical components and circuit topology. Moreover, most of the ECM-based SOC observers overlook the uncertainties of model parameters, so the accuracy and robustness are limited.

Capacity is another critical indicator for the efficient management of VRB. All types of batteries to date are accompanied by significant capacity losses during the long-time running. In terms of VRBs, the capacity loss is attributed to two processes, i.e. the imbalanced ion diffusion across membrane and the gassing side reactions during charging at both half-cells [28,29]. A merit of the VRB however, is that almost all of the capacity loss can be rejuvenated by remixing the electrolytes from two half-cells. Unsuitable cell design and abusive operation leads to side reactions in the negative half-cell, which further causes the irreversible capacity loss which cannot be simply restored by remixing the electrolytes. The side reactions however can be minimized by isolating the negative half-cell electrolyte and controlling SOC within a certain range. In this regard, the accurate monitoring of capacity loss is critical for the long-term VRB operation as it helps to decide when to start the re-balance treatments. From the view of model-based state monitoring, the capacity loss is also a critical uncertainty prohibiting the accurate estimation of other battery states, as it is involved in the state-space formula and cannot be updated easily [30,31].

To date, the capacity loss of VRB is majorly simulated with mathematical models [32–37]. The hydrogen evolution [32] and oxygen evolution [33] were modelled by considering the conservation of mass, charge, energy and momentum. Further, Skyllas-Kazacos and Goh [34] modelled the vanadium ion diffusion across the separator in seeking to simulate the capacity loss over extended cycling tests. A comprehensive mathematical model was then proposed combining the processes of both the ion diffusion and side reactions [35]. Most recently, a mathematically determined capacity fading factor was included in the battery model and the sliding mode observer was used for the simultaneous monitoring of SOC and capacity loss of the VRB [38]. The aforementioned methods are quite insightful for the capacity decay analysis and cell design optimization. However, these models require accurate calibration of parameters which are highly dependent on the physicochemical properties of VRB, thus it is difficult to model the capacity loss accurately within a wide range of working scenarios. In light of this, the real-time monitoring of capacity loss should be further elaborated to operate VRB with enhanced safety and efficiency.

This paper aims to address the above challenges and propose a model-based observer for the online monitoring of SOC and capacity loss of VRBs. A novel autoregressive exogenous (ARX) model is proposed to capture the dynamics of the VRB. The ARX model is free from the restrictions brought by the physical interpretation of model parameters and enjoys much higher flexibility on model order and structure. The order of ARX model is scrutinized based on the trade-off between model accuracy and complexity. The offline parameterization based on a genetic algorithm (GA) and the online parameterization based on recursive least squares (RLS) are investigated and compared in terms of modelling accuracy and robustness. Based on the parameterized ARX model, an H-infinity observer (HIO) is formulated to observe the SOC and simultaneously detect the capacity loss of the VRB in real time. Lab-scale experiments are carried out to verify the proposed method in terms of accuracy, convergence and robustness.

The rest of the paper is organized as follows. The proposed ARX model and the associated model parameterization methods are introduced in Section 2. The HIO-based observer for SOC estimation and capacity loss detection is presented in Section 3. Details of lab-scale experiments are presented in Section 4. Experimental results are discussed in Section 5, and the main conclusions are drawn in Section 6.

2. Autoregressive exogenous modelling

2.1. State of charge

The SOCs of each half-cell of VRB are different due to the occurrence of electrolyte imbalance. Strictly speaking, monitoring the SOC of each half-cell as done in Ref. [10] is required to know the real charge state of the VRB system. However, this is relatively complicated to be adopted in the practical BMS in the current stage. Instead, an overall SOC is defined in this paper from the engineering prospective, just like the OCV is used to indicate the overall SOC in the commercial VRB system.

Instead of using the theoretical SOC as involved in Nernst Equation, a new definition of SOC is proposed in this paper from the pure engineering prospective. The following definitions are firstly given to ease the description.

Definition 1. A cell is fully charged when its voltage reaches the upper cut-off voltage under the lower cut-off current. In this paper the upper cut-off voltage and lower-cut-off current are defined as 1.65 V and 1 A cm^{-2}, respectively. Under this definition, the cell is charged with a current density of 50 mA cm^{-2} up to 1.65 V, and then charged with the voltage maintained at 1.65 V until the charge current drops to 1 A cm^{-2}. The cell SOC is defined as 100% under this condition.

Definition 2. A cell is fully discharged when its voltage drops down to the lower cut-off voltage under the nominal load current. In this paper the lower cut-off voltage and nominal load current are defined as 0.9 V and 50 A cm^{-2}, respectively. Under this definition, the cell is discharged with a current density of 50 mA cm^{-2} to 0.9 V and at this condition the SOC is defined as 0%.

Definition 3. The capacity of a cell is the maximum number of ampere-hours that can be drawn from the cell before it is fully discharged at the defined temperature, starting with the cell fully charged.

The SOC is defined as the percentage of remaining capacity with respect to the maximum capacity. The dynamics of SOC can be written as: