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Development and perspective in vanadium flow battery modeling

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HIGHLIGHTS

- VFB modeling is of great significance for battery improvement.
- Modeling approach from macro scale to molecular/atomic scale was described.
- Modeling application from market level to material level was discussed.
- Models at the cell and material level play key roles in VFB research.

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ABSTRACT

Vanadium flow battery (VFB) is a promising candidate for large scale energy storage applications. Some critical challenges of VFB technology, especially for the issues unavailable via the experimental research, have motivated the use of VFB modeling, which can perform more efficient battery optimization than the extensive laboratory testing. Thereby, VFB modeling is quite necessary for the battery research. Based on the research scalability, the modeling approach in this review can be roughly grouped into three categories: macro approach, micro approach, and molecular/atomic approach. The modeling applications for VFB prediction can be classified into four levels: market, stack and system, cell, and material, presenting a decreasing scalability. The modeling approach and the modeling application along with their effectiveness and limitations in VFBs are discussed. A modeling perspective is also provided, highlighting the key role of the models at the cell and material level in battery research, and outlining the future direction in battery modeling for the VFB commercialization.

Contents

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1. Introduction

Global population growth and continuing industrialization drive an increasing demand for energy. As an alternative to conventional energy, renewable energy is a promising candidate due to its sustainability and diversification. In order to promote the development and application of renewable energy, numerous countries have planed the extensive deployment of clean energy [1–5]. However, the random and intermittent nature of renewable energy makes it quite challenging for the widespread applications. The electricity energy storage (EES), which is capable of storing and releasing electricity temporarily, is available to solve those problems [6]. As one kind of EES technologies, flow batteries (FBs) have efficiency, cost, cycle life, safety advantages and have been widely used for large scale energy storage. To date, a wide variety of FBs including all-vanadium [7], iron–chromium [8], bromine–polysulfide [9], zinc–cerium [10], zinc–bromine [11] have been successively proposed and developed. Due to the inhibition of cross contamination by employing the same chemical element (vanadium) as both positive and negative electrodes' active species, the vanadium flow battery (VFB) becomes the most promising candidate for large scale energy storage. It has been successfully deployed in an extensive range of applications such as load leveling and peak shaving, uninterruptible power supply, emergency backup and facilitation of wind and photovoltaic energy delivery [12].

Over the last two decades, a considerable number of demonstrative projects in VFBs have taken place in Austria, Canada, Japan, China and Thailand [13]. The battery performance has been significantly improved by exploring the key materials (membrane, electrode, and electrolyte) [14–22] and optimizing the VFB system (battery/stack structure and operation conditions) [23–25] in recent years, and the VFB system cost is lowered accordingly, which drives the fast commercialization and industrialization of VFBs. However, some critical challenges still remain, such as vanadium ions crossover through the membrane, the resultant self-discharge and capacity loss over repetitive cycling, unwanted side reactions, uneven electrolyte concentration, poor stability and solubility of electrolyte, default heat management, improper operation conditions and scale-up for the VFB. With regard to these problems, the VFB optimization including materials or battery/stack structure design and operation conditions is of great importance. Whereas, achieving the objective via extensive laboratory testing is inefficient or even difficult for some issues. In pilot studies, modeling can be a promising candidate, which has commonly been used in fuel cells [26]. By modeling, the VFB optimization can be made more efficient and accessible due to the cost-effective and time-saving characteristics. Thereby, VFB modeling is quite necessary for the battery research.

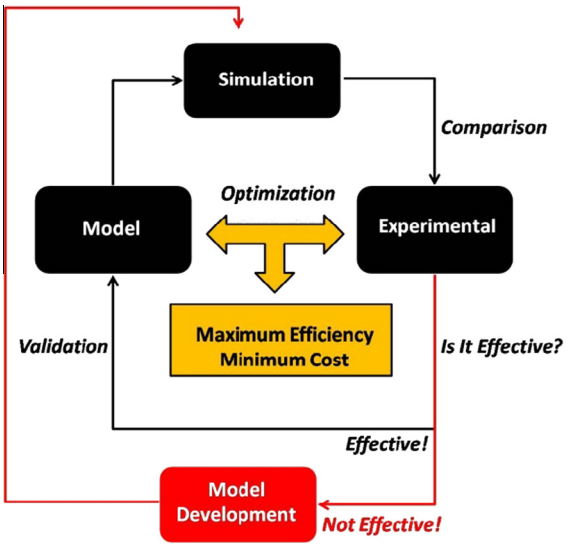

Fig. 1. The procedure for VFB improvement via modeling.

Fig. 1 shows a schematic of the procedure for VFB improvement via modeling. Referring to the schematic, the approach generally begins with a model. The initial model would be validated by comparing the simulations with experimental data, which would be used to develop and refine the detailed model until its simulations became effective when validated against experimental data. The most effective model should reflect the issues addressed, satisfy the computational requirement and provide with sufficient accuracy. The effective model, may be a cell model or a system model, can be simulated in the most efficient way and would then be employed as an instrumental tool for optimizing structure and operation conditions, and controlling or monitoring the VFB system. By the optimization strategy derived from the simulations, ideally, the eventual goal of the process would develop a VFB system with maximum efficiency and minimum cost. In this regard, model development is of great significance for battery improvement.

Models for VFB vary widely in terms of computational complexity, research scalability and accuracy of predictions. The model development for VFB in this review is summarized in Fig. 2, in order of a decreasing scalability, which presents the modeling approach from the macro to the molecular/atomic scale, and the modeling application of the approaches from the market level to the material level. The macro approach usually relates to the methods applicable for macroscopic phenomena in a unit cell, VFB stack/system and the market. To a smaller scale, it holds for micro approach, which describes the problems in a micro structure, such as a pore electrode, a pore membrane. At the most fundamental scale, it is the molecular/atomic approach, which can be used to probe into the electron structure and nature of the materials at the molecular/atomic scale. For modeling application, at the market level, the basic issues such as cost, safety and life of the VFB system are the main concerns. Different modeling approach associates with different application. At the stack and system level, the models are widely used as the monitoring, controlling and management tool for VFB. The detailed physicochemical processes