Journal of Energy Storage 15 (2018) 133–144

Contents lists available at ScienceDirect

Journal of Energy Storage

journal homepage: www.elsevier.com/locate/est

Mechanical modelling and simulation analyses of stress distribution and material failure for vanadium redox flow battery

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ARTICLE INFO

Article history:
Received 21 September 2017
Received in revised form 7 November 2017
Accepted 9 November 2017
Available online xxx

Keywords:
Vanadium redox flow battery
Stress distribution
Material failure
Mechanical model
Simulation analyses

ABSTRACT

During the operation of vanadium redox flow battery, the cell stack can suffer from electrolyte leakage and material failure that significantly affect the overall performance of the battery, provided that the stack is improperly designed and assembled. In order to manufacture more reliable battery stacks without undergoing electrolyte leakage and mechanical failure, the stress distributions on all key components of the stack need to be known. In this study, three-dimensional mechanical models are developed to perform simulation analyses on stress distribution for the cell stacks. Stress distributions on key cell components under specified sealing gasket designs, assembling forces and number of cells in a stack are investigated for the single cell and multi-cell stacks, while potential material failure and damage for the stack components are also analyzed in accordance with maximum stress criterion and von Mises yield criterion depending on the material of the components. Simulations results successfully demonstrate the stress distribution and magnitude in specified stack design and assembly condition, and highlight the importance of mechanical analyses in developing flow battery stacks with superior sealing and mechanical performance for long-term use.

1. Introduction

Benefit from the widespread use of renewable energy sources such as solar and wind, electrochemical energy storage technologies have been greatly developed in recent years aiming to tackle the problems of poor stability and reliability introduced by the intermittent nature of renewable energy generations on the grid integration as well as to store excessive energy from the renewables for the demand of stationary applications. Of all the electrochemical energy storage candidates, the vanadium redox flow battery (VFB) initially proposed by Skyllas-Kazacos and co-workers in the mid-1980s has received extensive attentions and yet reached commercial fruition [1–4]. Distinguishing from secondary batteries and other flow batteries, the VFB employs vanadium sulfate as electrolytes in both half-cells that avoids the issue of cross-contamination while taking advantages of the electrolyte circulation and external electrolyte storage reservoirs to design the power output and capacity separately. As such, the great potential of the all-vanadium redox flow battery in large-scale energy storage utilization integrated with wind turbine or photovoltaic has been successfully demonstrated in a number of applications ranging from kW/kWh to MW/MWh throughout the world [5].

Despite successes achieved in real-life applications, certain technical challenges and engineering issues affecting battery overall performance and lifetime still bother the flow battery manufacturers [6]. On typical concern is with respect to the electrolyte leakage (both internal and external) and material failure for the flow battery stack. In practice, most of the flow battery manufactures conventionally employ sealing gaskets or O-rings in combination with compressive forces exerting on the thick end-plates to seal the cell stack. Although the stack can exhibit accredited sealing performance in the testing, it is still prone to suffer from electrolyte leakage during long-term operation. Alternatively, some flow battery developers such as Cellstrom and SEA in Austria have successfully fabricated small welded stack modules and integrated them into their flow battery application systems [7], but scaling-up the welding process for large stack fabrication still has not come to fruition owing to certain limitations of the welding equipment in processing large stack design as well as the consideration of cost reduction. Fundamentally, the electrolyte leakage and material failure are caused by uneven stress distribution in the stack that, in combination with electrolyte surface tension, gives rise to the capillary effect, as well

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https://doi.org/10.1016/j.est.2017.11.011

as overlarge stresses in excess of the material strength that closely associate with the mechanical properties of the stack component material (e.g. Young's modulus) and the magnitude of external assembling forces. Particularly if any stack component receives excessively large stresses concentrating on certain areas, the plastic deformation or cracks can occur and potentially exacerbate the electrolyte leakage, along with any existing non-uniform stress distribution on the stack. It is therefore vital for each component of the cell stack of the flow battery to receive an appropriate mechanical stress in terms of both magnitude and distribution from the external assembling load that, to the greatest extent, avoids the material failure and electrolyte leakage. For this purpose, stress analyses for the cell stacks should always be performed prior to the design and fabrication of the stack, as it can comprehensively reveal the stress distribution in the stack and mechanical responses of all stack components.

In literatures, there are already some relevant mechanical studies reported for electrochemical energy storage systems. For instance, simulation analyses of the stress distribution for fuel cells have been recently described by Cruz [8] aiming to investigate the mechanical behavior of the fuel cell stack components. In order to improve sealing effect and avoid gas leakage, in addition, different sealing designs for the fuel cell have also been applied to investigate the stress and strain of the cell [9–11]. Other than fuel cells, stress analyses for lithium-ion battery have also been studied. While Fu et al. studied the mechanical stress generation and dimension of the lithium-ion battery to address the issues of disorder and fracture of the electrodes [12], the mechanical behaviors of lithium-ion battery were presented by Pan et al. through representative volume element specimens [13]. Besides, cylindrical lithium-ion battery cells were investigated by both mechanical testing and finite element simulation to explore the mechanism of deformation and fraction of the cell [14–16]. All these reported mechanical simulation studies for electrochemical energy storage systems successfully demonstrate the importance of mechanical analysis in system design and optimization. For vanadium flow batteries, however, all reported multi-physics simulation studies have focused on either the principles of electrochemical processes [17–26] or the cell design and operation conditions such as the thermal effect [27–31], the flow field [32,33] and shunt current [34–38], while no work concentrates on mechanical analyses of the stack design and assembly. Hence, performing a mechanical simulation to analyze the stress distribution in the cell stack of the VFB is an urgent task for flow battery researchers and engineers as a means to optimize the stack design and assembly.

In this study, three-dimensional mechanical models for the VFB cell stacks are developed and solved by finite element methods. Stress distributions on key components under specified sealing gasket designs and clamping forces are investigated for both a single cell and multi-cell stacks. Based on the stress distribution results, potential material failures for the stack components are analyzed by introducing maximum stress criterion and von Mises yield criterion applicable to brittle material and ductile material respectively. Simulation results demonstrate that the stress distribution and magnitude in the cell stack highly depend on the stack design and assembly condition, while also highlighting the importance of mechanical analyses in developing VFB stacks with superior sealing property and mechanical performance for long-term operation.

2. Finite element model

2.1. Cell geometry

Stress distributions on the cell stack of the VFB are analyzed by using COMSOL Multiphysics in this study. The finite element analysis model is constructed based on the VFB cell and stacks designed in our laboratory. In Fig. 1(a), all essential components required to assemble a single cell are illustrated, and the dimension of each component can be found in Table 1. Note that the end plate is designed slightly larger than the flow frame, so spring loaded bolts can be fastened at the holes on the end plates to assemble the cell or the stack through compression. In addition, simple flow channels are designed on the flow frame while the gaskets are also placed between adjacent components to seal the cell stack.

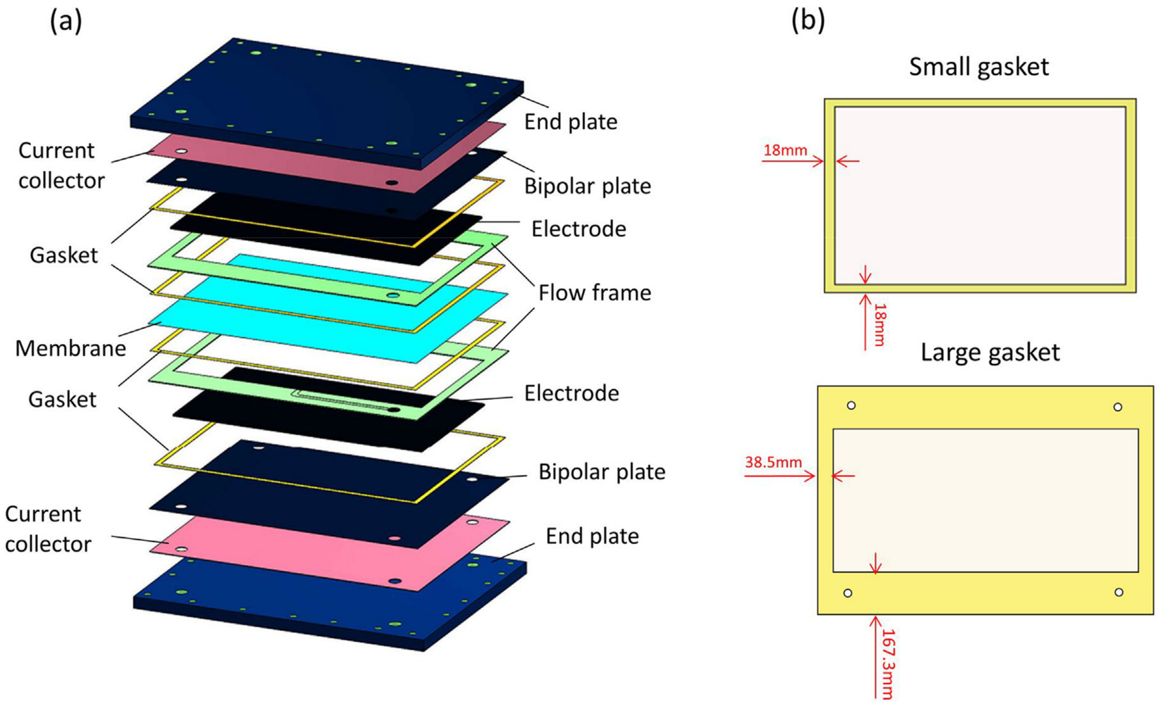

Fig. 1. (a) Single cell assembly components (b) Illustration of small and large gasket designs.