A coupled three dimensional model of vanadium redox flow battery for flow field designs

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ABSTRACT

A 3D (three-dimensional) model of VRB (vanadium redox flow battery) with interdigitated flow channel design is proposed. Two different stack inlet designs, single-inlet and multi-inlet, are structured in the model to study the distributions of fluid pressure, electric potential, current density and overpotential during operation of VRB cell. Electrolyte flow rate and stack channel dimension are proved to be the critical factors affecting flow distribution and cell performance. The model developed in this paper can be employed to optimize both VRB stack design and system operation conditions. Further improvements of the model concerning current density and electrode properties are also suggested in the paper.

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1. Introduction

ESS (Energy Storage System) technology based on electrochemical reactors is getting more attention in R&D and product commercialization [1–14]. VRB (Vanadium redox flow battery) system, with its advantages of high energy efficiency, long cycle life and flexible capacity design, is one of the promising ESS technologies for storage of renewable energy and stabilization of local grid electricity supplies [1–9]. Several VRB systems have been installed for product demonstration and field trials. However, their performance, lifetime and efficiency need to be improved significantly prior to VRB commercialization. Therefore, many scientists and engineers focused on fundamental studies of VRB electrochemical reactions to improve the system performance and lifetime [15–24]. Among these scientific studies, computational simulation is a powerful tool to reveal the nature of electrochemical reaction of VRB cell reactor and to save tremendous experimental work.

Over the last decade, numerical modeling of VRB system has been researched by many groups and simulations of flow-through porous electrode cell structures of VRB are discussed in detail [1,25–32]. M. Vynnycky built a 2D time-dependent single-phase isothermal model with single cell to optimize VRB operation condition [1]. A. A. Shah et al. proposed dynamic models of VRB system

and studied the effects of gas evolution, electrolyte flow rate and current density on cell performance [25–29]. While D. You investigated the effects of porous electrode thickness ratio on the current density distribution and a two-dimensional model of a single cell was developed to predict the cell performance [30]. A dynamic thermal model based on energy conservation was established by A. Tang and M. Skyllas-Kazacos to simulate the VRB stack temperature distribution characteristics with different stack structures [31].

Recently, Q. Xu et al. focused on numerical investigations of serpentine and parallel flow field designs of VRB cells and studied the cell performance for the different flow fields [32]. Compared to the two flow fields, the interdigitated flow field is a key technology to distribute electrolyte with less fluid pressure drop than the serpentine one and more efficient mass transfer than the parallel one. In this paper, a 3D stationary model of interdigitated flow field is proposed to simulate the distribution patterns of electrolyte fluid flow, cell's voltage and current density in terms of stack structure and electrolyte flow rate. Based on the simulation results, stack design parameters and operation conditions are optimized to improve both VRB performance and system efficiency.

2. Model development

2.1. Geometric model building

The theoretical model of VRB is based on a 3D single cell structure as depicted in Fig. 1, which is composed of current

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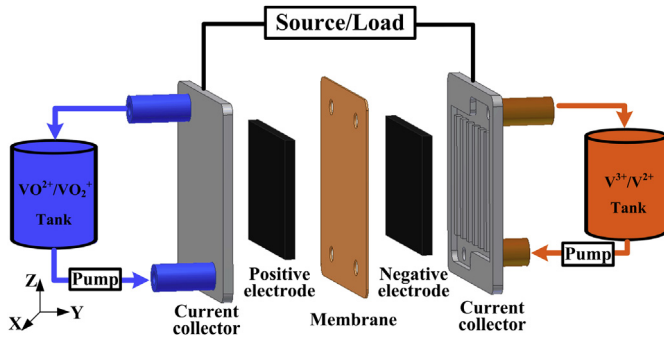E-mail addresses: yincong@dongfang.com (C. Yin), tanghao@dongfang.com (H. Tang).

Fig. 1. A schematic of an all-vanadium redox flow battery system.

Table 1
Default parameters of the VRB cell's geometric structure.

Symbol	Parameter	Value
a	Channel width	1.5 mm
b	Channel height	1.5 mm
c	Land width	2 mm
d_1	Porous electrode thickness	2 mm
d_2	Membrane thickness	0.5 mm
d_3	Current collector thickness	2.5 mm
m	Width of porous electrode	7 mm
n	Length of porous electrode	10 mm

collectors, porous electrodes and a proton exchange membrane. Electrolyte solution containing vanadium ions of different valences, V^{2+}/V^{3+} for the negative electrode and VO^{2+}/VO_2^+ for the positive electrode, are circulated into the cell stack by liquid pumps respectively. The main half-reactions of the two electrodes for VRB are as follows:

Negative electrode: $V^{3+} + e^- \Leftrightarrow V^{2+}$
Positive electrode: $VO^{2+} + H_2O \Leftrightarrow VO_2^+ + 2H^+ + e^-$
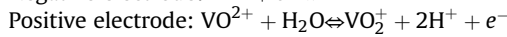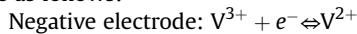
As the geometric size of a regular VRB cell is too large for computational modeling, a simplified 3D model is built in this paper as shown in Fig. 2, including current collectors with inlet and outlet channels, porous electrodes for positive and negative half-cells respectively, and an ion exchange membrane to separate the two half-cells. The so-called interdigitated flow channels are depicted in Fig. 2(b), where the electrolyte solution is forced to flow through the porous electrode between the inlet and outlet channels with dead ends in the current collector. The default structural parameters of the cell model are given in Table 1.

2.2. Model assumptions

Several assumptions are applied to the present model and shown as follows:

(1) The electrolyte is considered as incompressible fluid and dilute solution when dealing with the fluid flow issues, as the volume change is too small and the ionic concentrations are sufficiently low.
(2) Side reactions such as hydrogen and oxygen evolution are not taken into account.

(3) Crossover of vanadium ions and water through the membrane is ignored.
(4) Temperature effect is neglected in the present model.

2.3. Governing equations

In order to describe the fluid flow inside the cell, the Navier–Stokes equations for incompressible fluid are used for the laminar flow in channel domains and the Brinkman equations are applied to deal with fluids in porous electrode, respectively. The momentum and continuity equations for laminar flow are as follows:

$$\rho\left(\vec{u}\cdot\nabla\right)\vec{u} = -\nabla p + \nabla\cdot\left[\mu\left(\nabla\vec{u} + (\nabla\vec{u})^T\right)\right] + \vec{f} \tag{1}$$

$$\rho\nabla\cdot\vec{u} = 0 \tag{2}$$

where ρ is the fluid density, $\vec{u}$ is the velocity, p is the pressure, $\vec{f}$ is the volume force vector and μ is the dynamic viscosity of the fluid.

And for the fluid flowing in porous media, the corresponding equations are:

$$\frac{\rho}{\varepsilon}\left(\vec{u}\cdot\nabla\right)\frac{\vec{u}}{\varepsilon} = -\nabla p + \nabla\cdot\left[\frac{\mu}{\varepsilon}\left(\nabla\vec{u} + (\nabla\vec{u})^T\right)\right] - \frac{2\mu}{3\varepsilon}\nabla(\nabla\cdot\vec{u})$$
$$- \left(\frac{\mu}{K} + Q\right)\vec{u} + \vec{f} \tag{3}$$

$$\rho\nabla\cdot\vec{u} = Q \tag{4}$$

where ε is the porosity, K is the permeability of the porous medium and Q is the mass source.

On the basis of velocity field simulation, mass balance for each species is given by the Nernst–Planck equation:
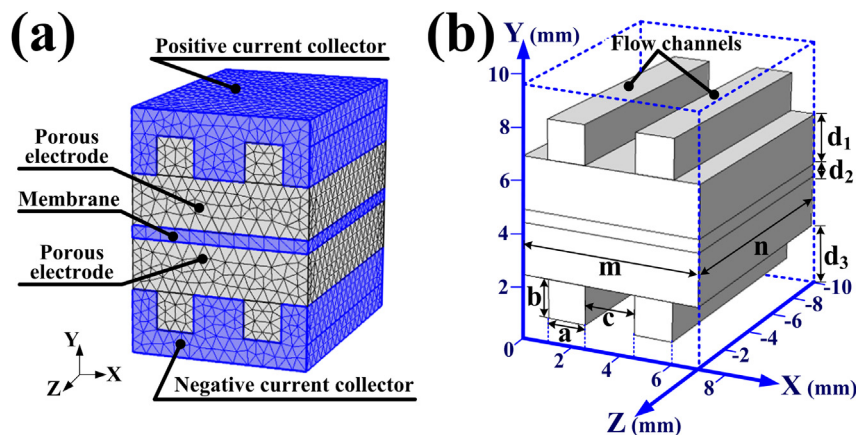

Fig. 2. The simplified 3D model of interdigitated flow channels for VRB cell composed of current collectors, porous electrodes and an ion exchange membrane. (a) The mesh building. (b) The detailed geometry.