Journal of Power Sources 279 (2015) 345–350

Contents lists available at ScienceDirect

Journal of Power Sources

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

Verified reduction of dimensionality for an all-vanadium redox flow battery model

A.K. Sharma [a, *], C.Y. Ling [a], E. Birgersson [a], M. Vynnycky [b], M. Han [c]

[a] Department of Chemical and Biomolecular Engineering, National University of Singapore, 117576, Singapore
[b] Division of Casting of Metals, Department of Materials Science and Engineering, Royal Institute of Technology, Brinellvägen 23, 100 44 Stockholm, Sweden
[c] Clean Energy Research Centre, Temasek Polytechnic, 529757, Singapore

HIGHLIGHTS

- Scale analysis of a two-dimensional VRFB model is carried out.
- A reduced zero-dimensional model is derived as a result.
- Two nondimensional numbers are found to govern the fidelity of model reduction.
- The reduced model is verified by comparing the charge–discharge curves.

ARTICLE INFO

Article history:
Received 19 November 2014
Received in revised form
22 December 2014
Accepted 4 January 2015
Available online 7 January 2015

Keywords:
Mathematical modeling
Transport phenomena
Scale analysis
Optimization
Control
Nondimensional number

ABSTRACT

The computational cost for all-vanadium redox flow batteries (VRFB) models that seek to capture the transport phenomena usually increases with the number of spatial dimensions considered. In this context, we carry out scale analysis to derive a reduced zero-dimensional model. Two nondimensional numbers and their limits to support the model reduction are identified. We verify the reduced model by comparing its charge–discharge curve predictions with that of a full two-dimensional model. The proposed analysis leading to reduction in dimensionality is generic and can be employed for other types of redox flow batteries.

1. Introduction

Recently, mathematical modeling and numerical simulations have come to play a key role in the understanding of transport phenomena in all-vanadium redox flow batteries (VRFBs). Detailed transport models for VRFBs usually consider changes in properties in time and/or space and, thus, consist of coupled non-linear partial differential equations (PDEs) that govern the conservation of mass, momentum, species, energy, and charge in the various layers (current collectors, electrodes, and membrane). One of the criteria based on which these models can be classified is the model dimensionality or the number of spatial dimensions considered: three- (3D) [1–5], two- (2D) [6–14], one- (1D) [15,16] and zero-dimensional (0D) models [17,18]. The associated computational cost for a system of PDEs decreases as the number of spatial dimensions is decreased. Because of the reduced computational cost, the lower dimensional models would be more suitable for wide-ranging parametric studies of a single cell, stack or system, real-time optimization and feedback control; in particular, the latter two require solutions within milliseconds [19]. There is thus a need to derive reduced dimensional models that can predict the cell behavior at a minimal computational cost while preserving the essential physics.

The model reduction from 3D to 2D is straightforward and does not require detailed analysis. The porous nature of the carbon felts and the membrane and the solid nature of the current collector allow for a reduction from three (x,y,z) to two dimensions (x,y)

* Corresponding author.
E-mail addresses: cheaks@nus.edu.sg, ashwini.ashwin@gmail.com (A.K. Sharma).

http://dx.doi.org/10.1016/j.jpowsour.2015.01.019
0378-7753/

because changes in the dependent variables in the spanwise direction (z) are negligible (see Fig. 1a and b); hence a 2D model ought to be able to capture the behavior of a 3D cell. However, further reduction in the dimensionality, i.e., 2D to 1D or 0D needs to be carefully analyzed. Although 0D models have been proposed in literature [17,18] as mentioned before, the authors did not justify or explain whether their models can indeed capture the behavior of a 2D cell.

In our earlier work on fuel cells [20–23], we employed scale analysis and asymptotic reductions to reduce the complexity of the governing equations and, therefore, their computational cost. The approach both preserves the essential physics and reduces computational cost. A similar approach has been exercised in our work on VRFB modeling [12,15]. In [15], two model reductions were proposed: first, the plug flow in the electrodes at the leading order and second, negligible species diffusion terms in the streamwise direction (y-direction in Fig. 1), whereas quasi-steady state behavior for typical VRFB operation was established in Ref. [12]. This paper, in essence, adopts a similar approach, i.e., we carry out scale analysis of a 2D model accounting for conservation of species and charge in a VRFB to derive a reduced 0D model (see Fig. 1b and c). The conditions when a 0D model can capture the behavior of a 2D cell are identified in the process.

The layout of the paper is as follows. First, the mathematical formulation is introduced in Section 2. Section 3 describes scaling arguments to support the model reductions from 2D to 0D. In Section 4, the results of the reduced model (0D) are verified against those of the full model (2D) and validated with experimental charge–discharge curves. The savings in computational cost in terms of memory usage and computing time are then discussed in Section 5. Conclusions are drawn in Section 6.

2. Mathematical formulation

We consider a transient 2D model (see Fig. 1b) accounting for conservation of species and charge in various functional layers of the battery: viz., current collector, electrodes, and membrane. For the sake of brevity, we summarize the full set of the governing equations, boundary and initial conditions in the following and refer to our previous work [12] for more details.

Governing equations.—we consider conservation of species and charge expressed as

$$\frac{\partial}{\partial t}(\varepsilon c_{\mathrm{i}}) + \nabla\cdot\mathbf{N}_{\mathrm{i}} = -S_{\mathrm{i}} \ (\mathrm{ne},\ \mathrm{pe}) \tag{1}$$

$$\nabla\cdot\mathbf{i}_{\mathrm{m}} = 0 \ (\mathrm{m}) \tag{2}$$

$$\nabla\cdot\mathbf{i}_{\mathrm{s}} = -S_{\mathrm{pot}} \ (\mathrm{cc},\ \mathrm{ne},\ \mathrm{pe}) \tag{3}$$

$$\nabla\cdot\mathbf{i}_{\mathrm{e}} = F\sum_{\mathrm{i}=1}^{n} z_{\mathrm{i}}S_{\mathrm{i}} \ (\mathrm{ne},\ \mathrm{pe}) \tag{4}$$

where the molar fluxes of species, $\mathbf{N}_{\mathrm{i}}$ and current densities, $\mathbf{i}$ are defined as

$$\mathbf{N}_{\mathrm{i}} = -D_{\mathrm{i}}^{\mathrm{eff}}\nabla c_{\mathrm{i}} - z_{\mathrm{i}}u_{\mathrm{i}}c_{\mathrm{i}}F\nabla\phi_{\mathrm{e}} + c_{i}\mathbf{u} \tag{5}$$

$$\mathbf{i}_{\mathrm{m}} = -\sigma_{\mathrm{m}}\nabla\phi_{\mathrm{m}}, \tag{6}$$

$$\mathbf{i}_{\mathrm{s}} = -\sigma_{\mathrm{s}}\nabla\phi_{\mathrm{s}}. \tag{7}$$

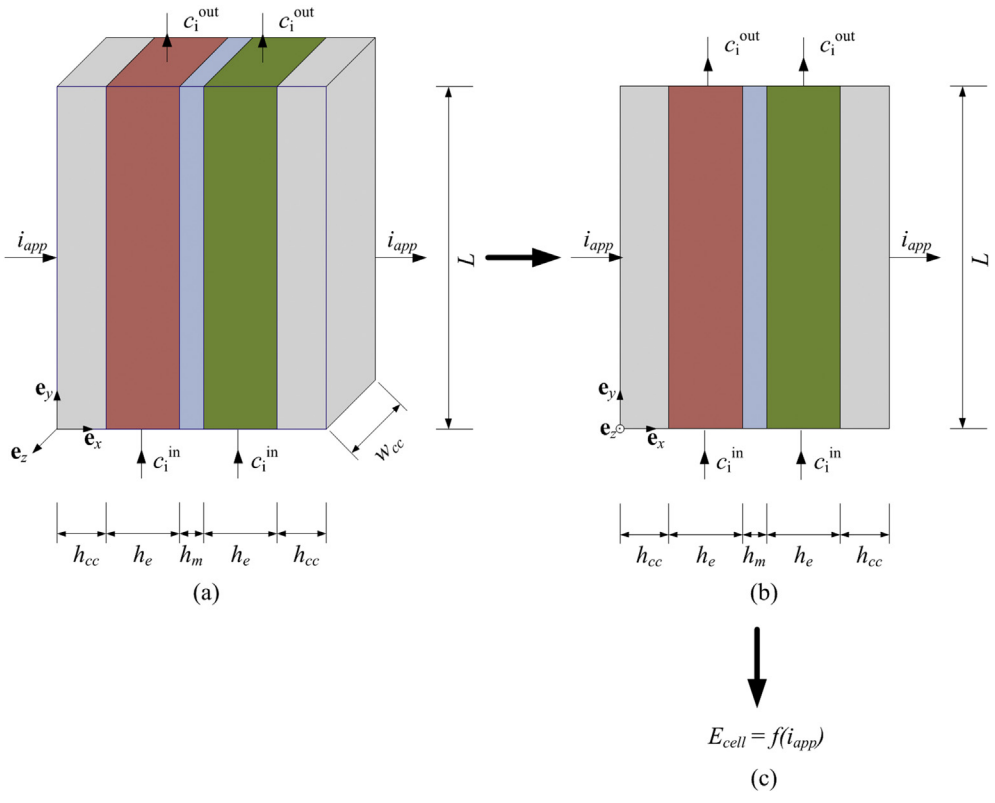

Fig. 1. A schematic of single cell vanadium redox flow battery with different number of spatial dimensions considered: (a) 3D model, (b) 2D model, and (c) 0D model.