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Flow simulation and analysis of high-power flow batteries

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HIGHLIGHTS

- Redox flow battery flow fields were modeled using CFD.
- High power density flow rates and cell areas up to 400 cm^2 were simulated.
- Pressure drops were quantified as a function of cell design.
- Correlations between slow transport and cell degradation were demonstrated.

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ABSTRACT

The cost of a flow battery system can be reduced by increasing its power density and thereby reducing its stack area. If per-pass utilizations are held constant, higher battery power densities can only be achieved using higher flow rates. Here, a 3D computational fluid dynamics model of a flow battery flow field and electrode is used to analyze the implications of increasing flow rates to high power density operating conditions. Interdigitated and serpentine designs, and cell sizes ranging from 10 cm^2 to 400 cm^2, are simulated. The results quantify the dependence of pressure loss on cell size and design, demonstrating that the details of the passages that distribute flow between individual channels and the inlet and outlet have a major impact on pressure losses in larger cells. Additionally, in-cell flow behavior is analyzed as a function of cell size and design. Flow structures are interrogated to show how and where electrode parameters influence pressure drops, and how regions where transport is slow are correlated with the presence of experimentally observed cell degradation.

1. Introduction

As the electricity share generated by intermittent sources such as solar and wind grows, increasing attention is being placed on energy storage technologies that can handle grid-scale demand. Flow batteries [1,2,3,4,5] have been proposed as a means of addressing grid scale needs [6,7,8] because their capacity can be increased simply by using larger active material storage tanks. However, these batteries are subject to a number of materials and engineering challenges that tend to increase system costs and inhibit realizability [8]. Many of the cost challenges can be addressed by moving towards higher power density stacks, which reduce the area and hence material required for a given power output. But, such a move requires special consideration of how higher power densities affect design parameters such as flow rates, electrode thicknesses and pumping losses. These considerations must include scalability, since industrial flow batteries may use cells with active areas on the order of 1000 cm^2 [5]. This paper considers the flow transport physics associated with the higher flow rates required for higher power densities.

Two flow transport processes particularly influence the performance of a flow battery cell. First, the pressure drop required to move reactants throughout the system is a load that reduces the system efficiency. Minimizing this pressure drop will allow more of the cell's energy to be devoted to useful work. Second, the velocity distribution within a flow field and electrode has a direct impact on mass transport to the reaction sites on the surface of the porous electrodes. For example, if a flow dead zone occurs within a porous electrode then mass transport will be supported only by diffusion

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and migration. This can significantly reduce the local current density relative to other regions where reactants are being actively supplied through convection. The presence of flow dead zones can also lead to localized degradation because these zones can foster local electrochemical or chemical conditions that drive unwanted processes (e.g., carbon oxidation). An example of such degradation in a 50 cm^2 variant of an experimental H_2/Br_2 flow cell [8,9] is shown below in Fig. 8a. Similarly, neutron imaging has indicated [10] that transport limitations occur around complex features in fuel cell flow fields. The importance of reactant transport in flow batteries motivates the need for a detailed understanding of fluid flow within these cells. Here, three-dimensional (3D) computational fluid dynamics (CFD) tools are used to advance this understanding.

The application of CFD modeling to flow batteries is limited, but the technique has been used to study flow through other electrochemical systems such as fuel cells [11,12]. For example, a series of studies have investigated transport in Proton-Exchange Membrane Fuel Cell (PEMFC) settings [13,14,15,16,17,18]. This body of work analyzed representative elements from PEMFCs, such as a set of two individual flow channels or an extracted section of a 3D cell geometry. Findings include the importance of 3D flow effects, analyses of where phase change in PEMFCs is important, and demonstrations of the ability to predict relationships between transport behavior and electrochemical performance. Because only representative cell elements were considered, however, pressure drops across entire cells and the influence of full flow field design parameters could not be assessed.

A second series of studies [19,20,21,22,23] used CFD techniques to simulate full 3D PEMFCs. These studies examined polarization curves, pressure drops, and a number of cell design parameters. Furthermore, a detailed review of how a series of 3D flow field parameters influence PEMFC performance was performed by Manso *et al.* [24]. Channel design, flow direction, channel length and number, channel cross section shapes, and baffle designs were all considered. For the most part, the active cell areas being considered in these full cell efforts were below 25 cm^2. The work of Kvesić *et al.* [22] was an exception, in that they simulated a 5 cell PEMFC stack with individual cell areas of 200 cm^2. Their study, however, invoked a lumped porous model in which the geometric details of the flow fields in each cell were not resolved. Full simulations of the large cell areas that are needed for industrial applications and high power densities, and the consideration of scalability, was not in focus.

While some analysis from PEMFC literature is directly applicable to Vanadium / Vanadium [25], Hydrogen / Bromine [8,9,26], and other redox flow batteries, important differences between PEMFCs and flow batteries exist. These differences include the use of single phase transport in many flow battery half cells, and they motivate the consideration of designs specific to flow battery requirements. While less common, CFD models of flow battery systems have been developed by a few groups. Latha and Jayanti [27] analyzed flow battery hydrodynamics using both experimental and 3D CFD analyses. They compared pressure drops and velocities in representative sections of ~40 cm^2 interdigitated and serpentine flow field designs, and particularly noted why these designs might be viewed differently from fuel cell and from flow battery perspectives. Brunini *et al.* [28] developed a 3D single channel model of a novel semi-solid variety of flow battery [29] in which both electrically conductive and solid, ion accepting particles are suspended in a transported liquid medium. Their model was used to investigate how the dependence of the voltage on the state-of-charge influences system performance. The group also developed a 2D semi-solid flow battery CFD model [30].

This paper seeks to build upon existing flow battery modeling literature by considering full cell designs with their associated flow delivery and removal passages, and by considering the cell areas (up to 400 cm^2), scalability concerns, and flow rates that are relevant for industrial high power density operating conditions. This introduction serves as Section 1 of the paper. Section 2 describes the different flow field designs that are considered. The governing equations and computational infrastructure used for the CFD calculations are presented in Section 3. Computational results are shown in Section 4, and the paper's conclusions are summarized in Section 5.

2. Simulated cases

The cases simulated in this work are variants of the H_2/Br_2 cell studied by Cho *et al.* [8,9]. This cell was experimentally tested using both 10 cm^2 flow-through and 10 cm^2 and 50 cm^2 flow-by serpentine flow fields. Only the liquid (Br_2) side of the H_2/Br_2 cell is simulated here, since gaseous H_2 transport is expected to be less of a limiting factor than aqueous Br_2 solution transport.

Flow-through electrode designs can be used for flow batteries when low current densities are acceptable. In these flow-through designs, no channels are made in the battery flow fields and fluid travels across the entire area of the cell through the porous electrode. When current densities are low, flow rates are also relatively low and the pressure drops across flow-through designs are acceptable. Such designs are not appropriate for higher current densities, however, because higher flow rates are required. These higher flow rates can only be achieved in a flow through electrode with large pressure gradients that are driven by pumping systems which consume significant energy. This observation assumes that all flow in a flow-through design passes through an electrode of uniform porosity. More elaborate flow-through-like designs with spatially varying porosity have been proposed, but are not considered here.

The goal of minimizing pressure losses while supplying sufficient reactants to the electrode forces the consideration of flow-by designs. In these designs, open channels are cut into a solid plate that is placed adjacent to the electrode. The open channels provide fluid with lower resistance paths across the cell area. For example, Darling and Perry [31] experimentally compared the performance of a flow-through Vanadium flow battery with that of two flow-by designs. They found that the flow-through design would lead to significantly larger pressure drops than the flow-by designs as the cell size was scaled up toward industrial applicability. They also analyzed sensitivities to the transport phenomena that must be accounted for when switching between flow field designs.

Five flow-by designs that include three different cell sizes are simulated. Fig. 1 depicts the selected flow field geometries. The first two are serpentine channel designs: one 10 cm^2 design utilizing a single channel (Fig. 1a), and one 50 cm^2 design utilizing four channels (Fig. 1b). The channel in the 10 cm^2 serpentine design consists of 20 long passages connected by bends. The cross section of this channel is 1.016 mm high and 0.7874 mm wide. The spacing between channels is 0.853 mm. The dimensions of the 10 cm^2 serpentine design were chosen to mimic the experimental flow fields from Refs. [8] and [9], which employed hardware manufactured by Fuel Cell Technologies, Inc. The four channels in the 50 cm^2 serpentine design all consist of 11 long passages (44 in total) connected by bends. The cross section of each channel is the same, measuring 0.795 mm high and 0.795 mm wide. The spacing between channels is 0.795 mm.

The next three designs employ interdigitated flow fields (idffs). The dimensions of the interdigitated channels were chosen to ensure similarity with the serpentine hardware specifications. The first two interdigitated designs both have active cell areas of