GPU-enabled Pore-scale Transport Resolved Model for Vanadium Redox Flow Batteries

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Vanadium Redox Flow Batteries (VRFBs) (shown schematically in Fig. 1) have emerged as a viable grid-scale energy storage technology used in peak shaving applications due to their efficient cyclability and minimal cross-contamination effects. However, VRFBs suffer from having low energy and power densities, which can be resolved by improving electrode design [1]. As such, gaining insight into the effect of the electrode microstructure by using computer simulations is paramount in improving VRFB performance.

Existing volume-averaged models have been reported that treats the electrode/electrolyte matrix as a homogenous medium of uniform porosity [2]. By contrast, we have developed a pore-scale simulation for the VRFB that distinctly accounts for the separate electrode /electrolyte phases [3]. Our model requires no simplification or assumptions regarding the electrode morphology, and enabled us to carry out detailed studies into the effects of the precise electrode microstructure with unprecedented fidelity. A comparison between the two approaches is shown in plots of electrode overpotential in a smooth distribution of a volume-averaged model (Fig. 2a) and in a detailed 3D surface distribution using our pore-scale model (Fig. 2b).

The primary drawback of a pore-scale approach is the high computational resources required. Volume-averaged models are capable of simulating an entire 30mm × 3mm flow cell on a desktop computer, while we require parallel computations using multiple processors to simulate a 3mm×1mm subsection of the same flow cell. However, recent advancements in high performance computing have shown Graphics Processing Units (GPUs) to be an economical alternative to the traditional parallel computation techniques for solving problems in computational fluid dynamics [4].

We present in this work an application using GPUs to increase the speedup of our VRFB simulation in order to achieve realistic length and time scales not possible using traditional methods (Fig. 3). This work develops a finite volume method for the purpose of simulating electrochemical interactions at the pore scale of a VRFB. Effects of domain size, number of processors and threads on scalability and speedup are determined.

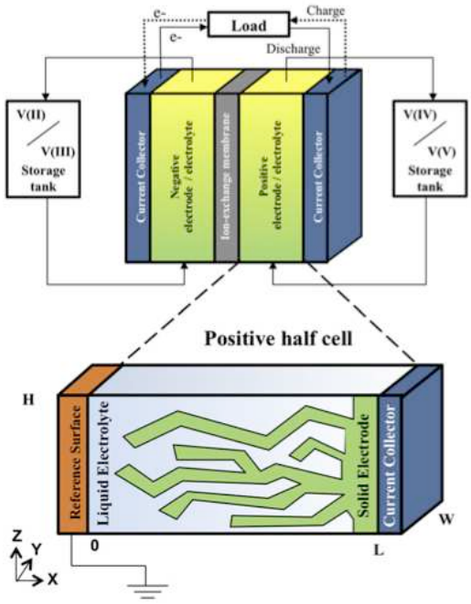

Fig. 1: Vanadium Flow Battery schematic, showing details of the electrode fibers [3]

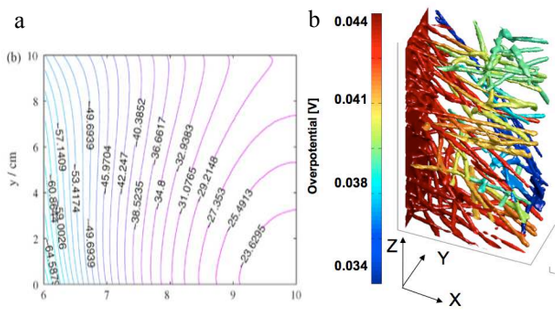

Fig. 2: Overpotential distribution plots for (a) volume-average model [2] (b) pore-scale model [3]

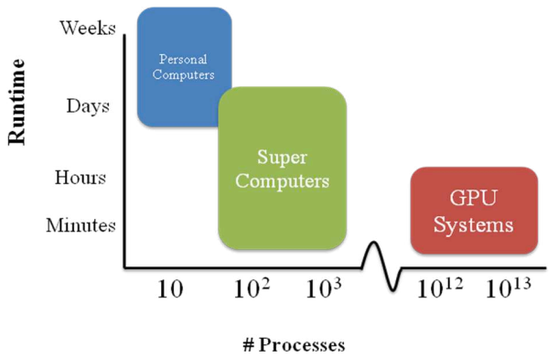

Fig. 3: Visual comparison of different methods for computational efficiency

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[4] Peter Zaspel, Michael Griebel, "Solving incompressible two-phase flows on multi-GPU clusters", *Computers & Fluids*, 2012.