Modeling the Vanadium Oxygen Fuel Cell

F.T. Wandschneider[1], M. Küttinger[1], P. Fischer[1], K. Pinkwart[1], J. Tübke[1], H. Nirschl[2]

[1]Fraunhofer-Institute for Chemical Technology, Pfinztal, Germany
[2]Karlsruhe Institute for Technology, Karlsruhe, Germany

Abstract

Introduction
Redox flow batteries are a promising technology for energy storage; the most prominent one being the all-vanadium redox flow battery (VRB). In this battery type, the energy is stored in liquid electrolytes that are pumped between tanks and cell stack and do not undergo a phase change. Due to its' relatively low energy density, it is mainly used in stationary applications. The vanadium oxygen fuel cell has been proposed [1, 2] for stationary, mobile and automotive applications that require higher energy densities. This is a combination of a VRB vanadium anode and a fuel cell air/oxygen cathode (Figure 1).

The use of COMSOL Multiphysics®
A two-dimensional stationary model of a vanadium oxygen fuel cell is developed in COMSOL Multiphysics®. The geometry is shown in (Figure 2). From left to right, there are a solid carbon electrode, a porous electrode with flowing liquid electrolyte solution, a Nafion® membrane, an intermediate chamber with another electrolyte solution, a Nafion® membrane with a catalyst coating on one side, a gas diffusion layer with flowing gaseous air and a second carbon electrode. On the right-hand side, there is a magnification of a part of the geometry to point out that the right membrane and the catalyst coating are modeled as two separate domains. The catalyst coating domain is modeled as a porous electrode to reflect the platinum catalyst particles that are partially covered by water. There is mass transport of hydrogen ions from the membrane and mass transport of oxygen molecules from the air within the gas diffusion layer. The oxygen reduction reaction generates additional water, leading to a degradation of the catalyst performance over time. A logistic function is introduced to the Butler-Volmer equation in order to model this degradation. The model can then be used in a semi-transient way.

The simulated data are validated against measurements of a vanadium oxygen fuel cell consisting of a single cell [3, 4]. The introduction of the logistic function leads to a good agreement between the simulated and the measured terminal voltages for a constant current discharge cycle (Figure 3), and the terminal voltages for different discharge currents. Further simulations with variations in the flow rate (Figure 4), surface area to volume ratio and electrochemical properties show that the low rate of the oxygen reduction reation has an extensive effect on the cell performance.

This work demonstrates the suitability of COMSOL Multiphysics® for the simulation of the

vanadium oxygen fuel cell. Further refinements of the model, like a more detailed description of the oxygen reduction reaction or the degradation mechanisms of the cathode, will allow a better understanding of the operating parameters within the cell. This will in turn lead to the improvement and optimization of further cell designs.

Reference

1. H. Kaneko, A. Negishi, K. Nozaki, K. Sato, M. Nakajima (1992) US Patent 5,318,865
2. J. Noack, T. Berger, K. Pinkwart, J. Tübke (2011) DE Patent 102011107185
3. J. Noack, J. Tübke, 3rd International Flow Battery Forum (2012) Munich, Germany
4. F.T. Wandschneider, M. Küttinger, P. Fischer, K. Pinkwart, J. Tübke, H. Nirschl: A coupled-phyiscs model for the vanadium oxygen fuel cell, submitted to the Journal of Power Sources
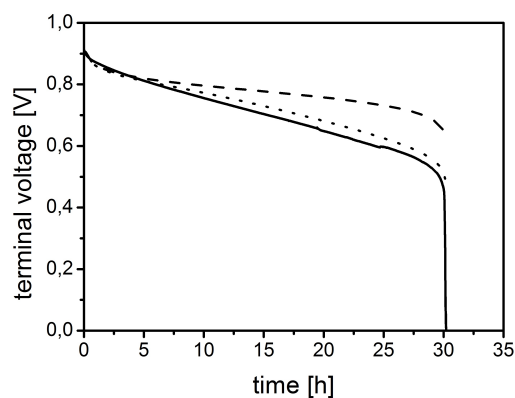
Figures used in the abstract
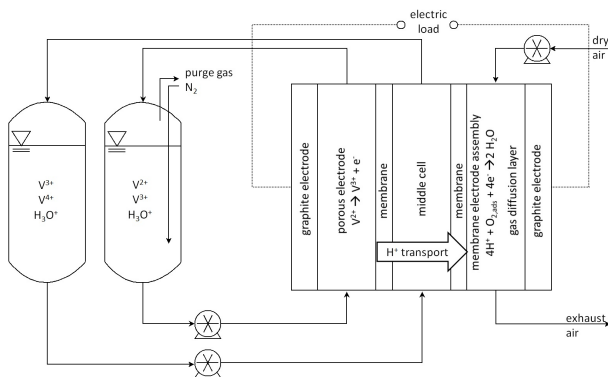
Figure 1: Process diagram of a vanadium oxygen fuel cell.
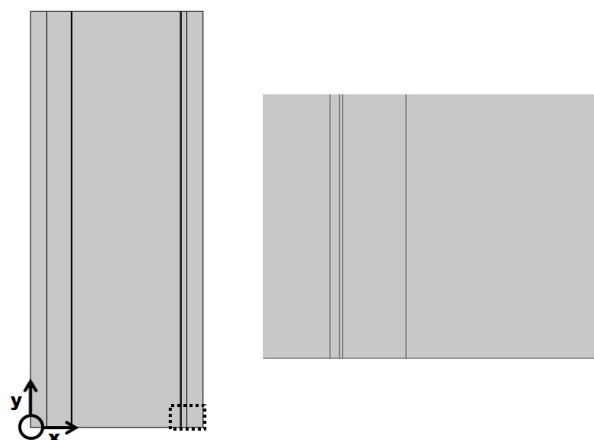
Figure 2: Model domains in COMSOL Multiphysics. Left-hand: whole geometry, right-hand: magnified part.

Figure 3: Comparison of experimental and simulated discharge process (measured data solid, simulated without logistic function dashed, simulated with logistic function dotted).
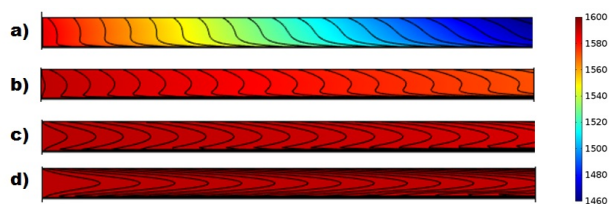
Figure 4: Surface plot of the local concentration [mol/m³] of V2+ ions in the anode with evenly distributed isolines. Volume flow rate of electrolyte a) 10 ml/min b) 33.3 ml/min c) 66.7 ml/min d) 100 ml/min with a current density of 75 mA/cm². The geometry has also been tilted 90° clockwise for better page fit. The inlet is to the left, electrode to the top, outlet to the right and the membrane at the bottom.