Mathematical Formulation of a PEM Fuel Cell Model

E. Robalinho[1], E. F. Cunha[2], M. Linardi[2], E. I. Santiago[2]

[1]Instituto de Pesquisas Energéticas e Nucleares - IPEN/CNEN, São Paulo, SP, Brazil; and Instituto Federal do Rio Grande do Sul - IFRS, Porto Alegre, RS, Brazil

[2]Instituto de Pesquisas Energéticas e Nucleares - IPEN/CNEN, São Paulo, SP, Brazil

Abstract

The idea of a friendly implementation of a mathematical formulation using specialist software was performed with the support of COMSOL Multiphysics® software with Chemical Reaction Engineering and Batteries & Fuel Cell Modules. The real problem of a Proton Exchange Membrane - PEM fuel cell modeling involves different scales, multiple variables and processes, coupling of solvers and experimental parameters. To solve this problem it is necessary an intensive use of memory and a robust formulation, which principal topics will be presented below. The first step is the calculation of potential of the cell by Nernst equation. The equations used in the distribution channels and porous media (Gas Diffusion Layer - GDL and Catalyst Layer - CL), are Navier-Stokes, Brinkman and continuity (Figure 1). The CL model represents the heart of the cell and uses the idea of agglomerates, and the equation of Butler-Volmer. Maxwell-Stefan and Darcy equations perform the mass balance; Laplace equation performs the charge balance. The initial conditions are presented in Figure 2. The boundary conditions were set up and linked to the anode and cathode current densities as indicated in the Figure 3. Experimental values of thickness of catalytic layer and the specific surface area were obtained from laboratories measurements. Finally, the values of concentration of gases, at agglomerate and reference value, the exchange current densities, the diffusivity and ratio of agglomerate were taken from the literature (Figure 4). Then, after this quick exposition about methodology, the data were evaluated using the solvers and post-processing features of COMSOL. The result of this implementation is a polarization curve that represents the fuel cell performance.

Reference

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Figures used in the abstract

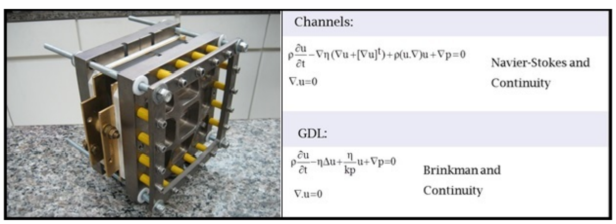

Figure 1: Real fuel cell and mathematical modeling of Channels and GDL.

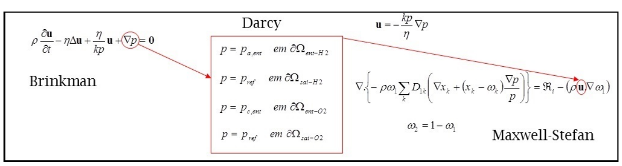

Figure 2: Getting the initial conditions from Darcy, Brinkman and Maxwell-Stefan equations.

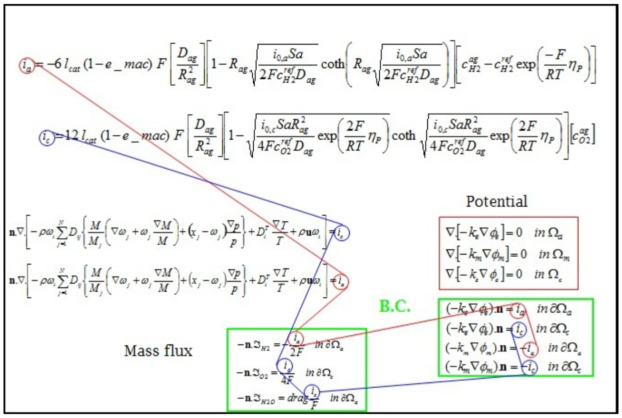

Figure 3: Boundary Conditions (B.C.) in coupling of the equations.

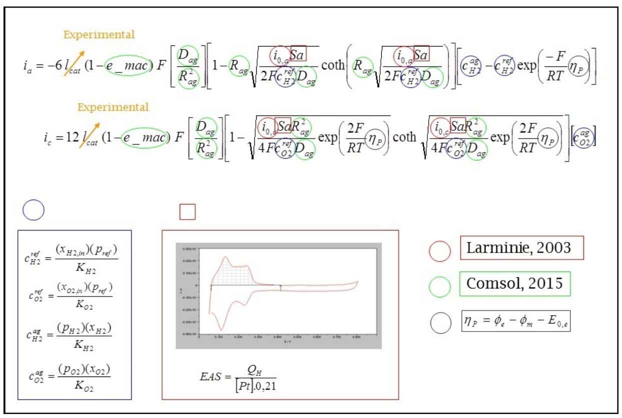

Figure 4: Experimental and literature parameters.