MODELING OF THE POTENTIAL JUMP AT ELECTRODE-ELECTROLYTE INTERFACE USING SINGULARITY DISTRIBUTION.

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Abstract

There is a jump in the electrical potential across the electrode/electrolyte interface of a fuel cell arising from electrochemical reactions. The magnitude of this jump is related to species concentration via Nernst's Law, and current density distribution due to electrochemical overpotentials. To provide a generalized numeric solution, a complete and detailed computational model should incorporate this phenomenon as part of the solution rather than specifying a priori as a boundary condition. A technique is proposed as a remedy to this non trivial problem. The new approach has an analogy from classical hydrodynamics where distribution of sources (or sinks) causes a jump in the velocity component normal to the surface on which the singularities are distributed. A doublet (or dipole) (Fig. 1) causes a jump in the potential field (Fig. 2) in a similar manner. The magnitude of the jump is proportional to the strength of singularity distribution. Based on these concepts, a dipole distribution at the electrode/electrolyte interface is used to model the jump observed in the electrical potential. The strength of the dipole singularities are calculated using Nernst's Law. Results, presented for fairly general cases, seem reasonable and capture the physical phenomenon observed in fuel cells.

A pseudo-empirical equation is used to calculate the magnitude of the potential jump for a typical solid-oxide fuel cell (Fig. 3). This, in turn, is used as a source term in the continuity equation for current density to obtain the desired results as shown in Fig. 3.
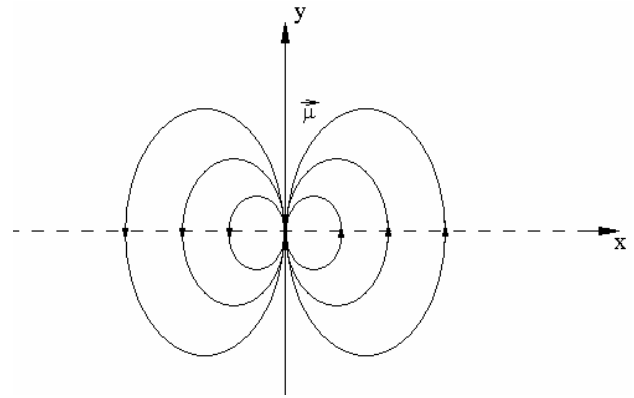
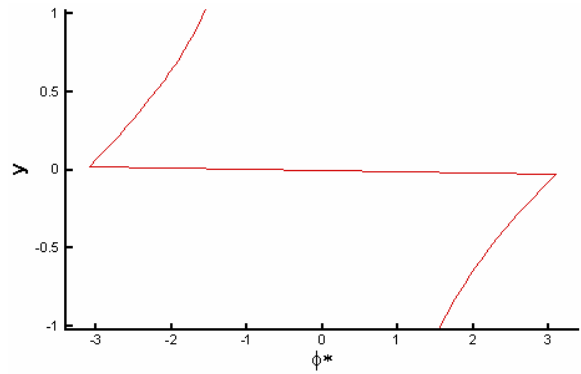Figure 1: Potential field around a dipole

Figure 2:Relative electric potential profile at x = 0 for a dipole distribution with a constant strength along the line x = 0.
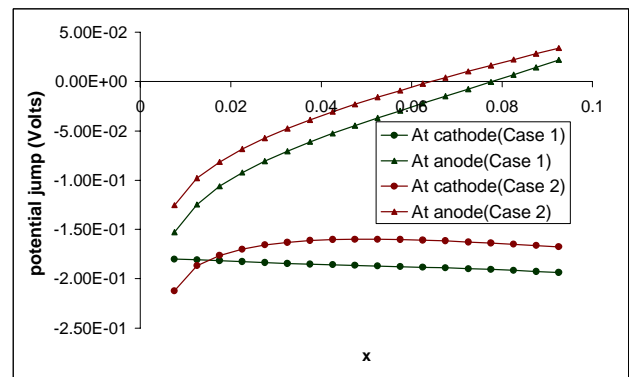

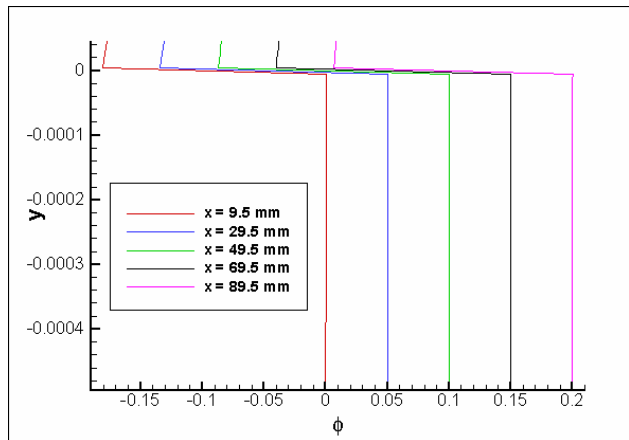Figure 3: Potential jumps on anode and cathode side calculated from species concentrations

Figure 4: Profiles of electric potential (Volts) at various x-locations