A Simulation of combined Magneto-Hydro-Dynamic and Multi Ion Electrochemical Systems

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Introduction

The aim of this work is to present a method for calculating electrode current densities distributions in an electrochemical reactor in presence of a magnetic field. If the fluid velocity is low, it is known that a magnetic field over the reactor can enhance the mass transport. This influences limiting currents and co-deposition rates if two metals are plated simultaneously. Hence the Magneto-Hydro-Dynamics (MHD) influences the electrodeposition process. Because magnetic materials are often plated electrochemically, there is a need in understanding the influence of the magnetic field on the plating process parameters.

Description of the Models

A general accepted model that describes an electrochemical reactor is the Multi-Ion Transport model [1]. This model expresses that the ionic fluxes are due to diffusion, migration and convection of the solvent. The convection can be calculated using the incompressible Navier Stokes (NS) equations [2]. If the reactor is placed in a magnetic field *B*, both the fluid flow and the ion transport are affected. The electric current density *J* between the electrodes induces a force F_B [3] on the fluid that is called Lorentz force :

$$\overline{F_B} = \overline{J} \times \overline{B}. \tag{1}$$

The movement of a charged particle in the presence of an electric field induces an additional migration current [3]. This behavior is often called the Hall effect [4]:

$$\overline{J}_{B,migr,k} = c_k z_k^2 u_k F\left(\overline{v} \times \overline{B}\right), \tag{2}$$

with c_k the ion concentration, z_k the ionic charge, u_k the ionic mobility, *F* the Faraday constant and *v* the local velocity.
The complete set of equations used to model the coupled system is:

$$-\overline{v} \cdot \overline{\nabla} c_k + \overline{\nabla} \cdot \left(D_k \overline{\nabla} c_k\right) + z_k F \overline{\nabla} \cdot \left(u_i c_k \left(\overline{\nabla} U + \overline{v} \times \overline{B}\right)\right) = 0,$$

$$\sum_k z_k c_k = 0,$$

$$\rho_m \left(\overline{v} \cdot \overline{\nabla}\right)\overline{v} + \overline{\nabla} p - \mu \Delta \overline{v} - \left(\sigma\left(-\overline{\nabla} U + \overline{v} \times \overline{B}\right) - F \sum_k z_k D_k \overline{\nabla} c_k\right) \times \overline{B} = 0$$

$$\overline{\nabla}.\overline{v} = 0, \tag{3}$$

with D_k the ionic diffusion coefficient, *U* the electric potential, ρ_m the density of the solvent, *p* the local pressure, μ the viscosity of the solvent and σ the local electric conductivity.

Reactor set up to validate model for the fluid flow

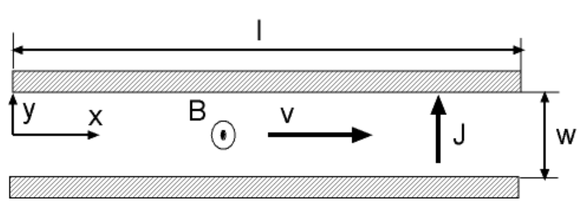

Figure 1

In figure 1 a typical parallel plate reactor is shown. Assume the inlet on the left and the outlet on the right. Between the inlet and the outlet fluid flows with velocity v. Over the reactor is a uniform magnetic field B perpendicular on the 2D geometry. The upper and lower boundaries are the electrodes. The current flows through the reactor between these electrodes due to electrode reactions. In order to verify the behavior of the MHD model the first computational experiment is to predict correctly the influence of the magnetic field on the Navier Stokes equations. To test this the setup is simplified. The electric current is put on a constant non-zero value in the whole reactor and a plug flow is imposed. The computed pressure field matches analytical results.

A second validation case for the influence of the magnetic field on the Navier Stokes equations is to simulate the Hartmann flow [5]. Computed results are in very good agreement with analytical results for different Hartmann numbers.

The set up for the simulated effects of the magnetic field on the mass-transport is as shown in Figure 1. The bath contains a $CuSO_4$/ H_2SO_4 aqueous solution. The pH is low to enhance the conductivity. At inlet and outlet zero pressure is imposed, so convection will only be due to the magnetic field. Bulk concentrations are imposed at inlet and outlet. The electric current densities are calculated by applying a Butler-Volmer equation on the cathode surface. This equation has been characterized by RDE-measurements when no magnetic field was applied. For different magnetic fields the current densities are computed in limiting and non-limiting situations. Calculations are compared with the Aogaki model [6].

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