A03-0171: Diffusion-Reaction-Limited Mass Transfer on the Surface of an Electrically Conductive Droplet

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16:20 - 16:40
📍 *Scottish Event Campus - Alsh 2*

Electrometallurgical processes are widely utilized in extraction and refining of metals [1]. Copper magneto-electrolysis [2] and aluminium smelting [3] are used to extract metals. Electroslag remelting (ESR) process is extensively used to refine metals [4]. A wide range of electrolytes such as copper sulphate-based, CaF_2-based, and sodium hexafluoroaluminate are used. Some of those processes (e.g. ESR) involve formation of metallic droplets which travel through the electrolyte. Electrochemical (Faradaic) reactions take place at the droplet-electrolyte interface aiming at refining of the metal.

Generally, the electrolyte operates at elevated temperature (~ 2000 K) and high electric current density (~ 10^5 $A.m^{-2}$) during refinement of the metal. As such, experimental analysis and measurements are quite difficult. Therefore, simulation tools can be effectively used to get insight into the invisible phenomena. Computational fluid dynamics (CFD) is a powerful technique that enables us to gain a deeper knowledge of the aforementioned processes. The obtained knowledge can be used to improve the technology, to minimize the failure rate, and to increase productivity.

Here, we propose a CFD model to study the electrochemical mass transfer at a droplet-electrolyte interface. The transport phenomena including flow, concentration, and electric current density fields are computed. A fully coupled model is developed to determine the concentration of the reactant as well as electric potential at the droplet-electrolyte interface. For that purpose, the interplay between the reaction kinetics at the droplet-electrolyte interface (Butler-volmer formula) and the diffusion-advection of reactant through the hydrodynamic boundary layer around the droplet is taken into account. The condition of the presences of excess of supporting electrolyte is assumed so that the migration transport of the reactant is ignored [5]. Of note, the droplet acts as both cathode and anode. Thus, the cathodic/anodic area on the surface of droplet must be computed that in turn depends on the intensity of the flow and the droplet size (more precisely Reynolds (Re) number).

In the present study, the system is composed of a copper droplet and the copper sulfate-sulfuric acid electrolyte for which kinetic and hydrodynamic properties (e.g. exchange current density, viscosity, etc.) are well-known [6]. Demonstratively, an example of calculations (Re = 40) including the velocity (u), the normalized concentration filed of the Cu^{2+} reactant (C/C_∞), and the electric current density (j) is shown in Figure 1. In the bulk of electrolyte, the concentration filed (C_∞), the velocity field (u_∞), and the electric field (E_∞) are given. Several droplet sizes (0.5, 2, 4 mm) under different flow regimes (Re = 0.2, 2, 20, 40 and 80) were examined. It is found that the intensity of the flow filed and the direction/strength of electric field in the bulk of electrolyte can significantly impact the amount of electric current (~ mass transfer) which flows through the droplet. Based on the modeling results, the mass transfer is limited mainly by reaction for the small droplet, whereas the role of diffusion becomes more potent with the increase of the droplet size.

Figure 1. Field structures are shown for the droplet with 2 mm diameter at Re = 40. In each contour the magnitude (colour scale) and the direction (equisized vectors) is illustrated. (left) velocity field, (middle) concentration field, (right) electric current density field.

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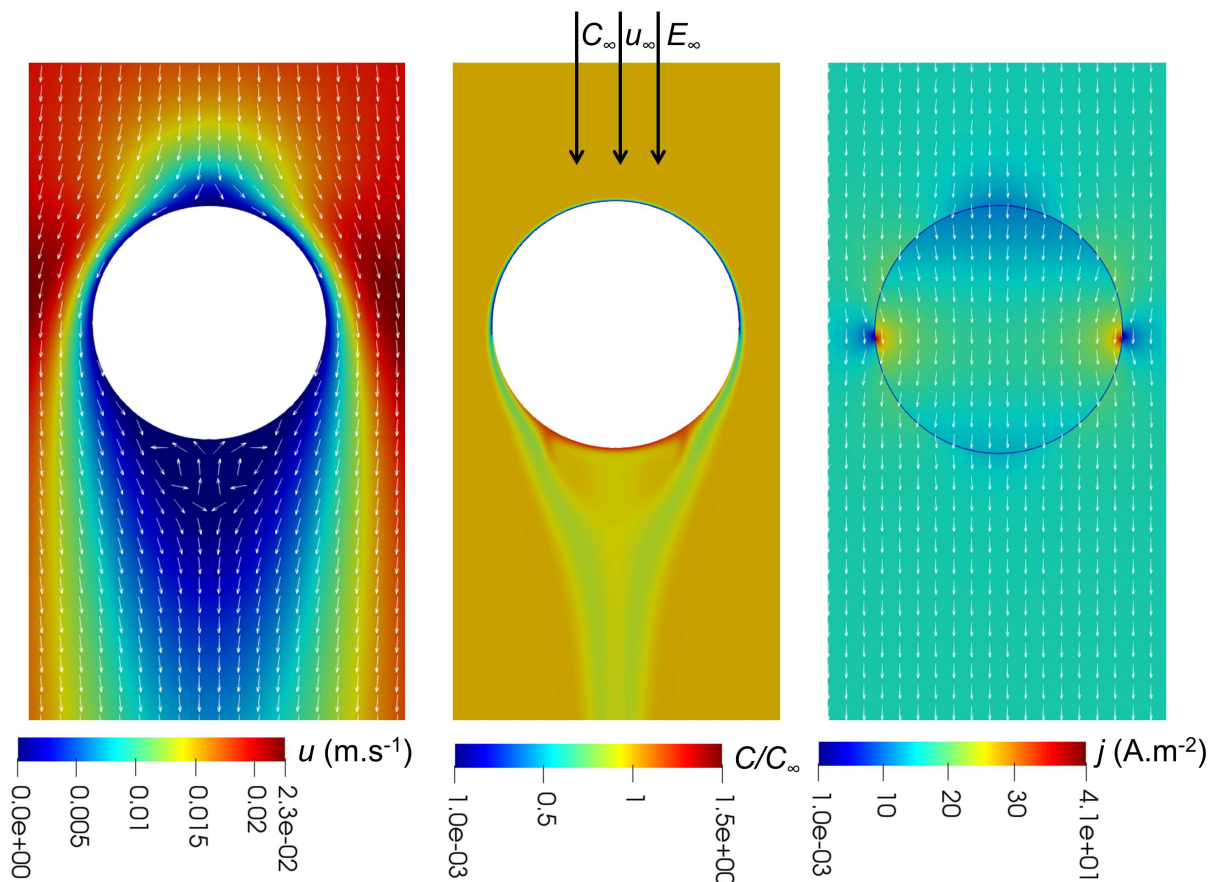
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