Transient Modeling of a Fluorine Electrolysis Cell Using COMSOL Multiphysics®

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Abstract

The design of the commercial fluorine electrolysis cells in operation in South Africa is based on technology dating essentially from the era before the proliferation of computer simulation software. The model reported here was initiated to generate a more fundamental understanding of cell operation, and to enable the rational optimisation possibility this may allow. COMSOL Multiphysics® was used to simulate a laboratory fluorine electrolysis cell which operates in the temperature range 80 °C to 110 °C with a nickel anode (Rudge, 1971: 7-14). The operational cell produces roughly 1 gram of fluorine gas per hour. The model geometry was set-up as 3D due to lack of symmetry in the applied Pauling cell (Pauling, 1957: 277) geometry. The Pauling cell uses two tubes joined at a 90 ° angle with an electrode in each tube. The CAD Import module was used to import the geometry of the relevant volume from the 3D design of the cell. Prior research has shown that secondary current distribution is representative of reality (Roustan & Caire, 1998) and was implemented using the Electrochemistry module with Butler-Volmer kinetics. The controlled temperature of the reaction tubes is included with isothermal boundaries using the Heat Transfer module. An Electrochemical Heating Multiphysics node was added to include Joule heating of the electrolyte. The overall reaction is the electrolysis of HF into H2(g) and F2(g). Electrolyte current density at the surface of the electrodes was applied to determine product gas flux. A Bubbly Flow, Laminar Flow interface from the CFD module (Pretorius, 2010) included the resulting mass and momentum transfer effects. Only the properties of fluorine phase (the heavier species) was specified. This simplification was justified by the simulacrum results which show negligible effects to electrolyte flow and current distribution by the hydrogen phase. Resulting mixing and temperature profiles of the cell may be investigated at different operation potentials. These simulacra are compared to voltammetry results of the laboratory and model are compared and presented. A good fit of the data is expected. This model, with confirmed accuracy, may be used to avoid unnecessary laboratory experiments with hazardous chemicals and aid in accurate scale-up procedures. An modeling result for an average current density of 12 A•m-2 on the working electrode predicts an overpotential of 0.02 V and fluorine production of 0.28 g•h-1.

Figures used in the abstract

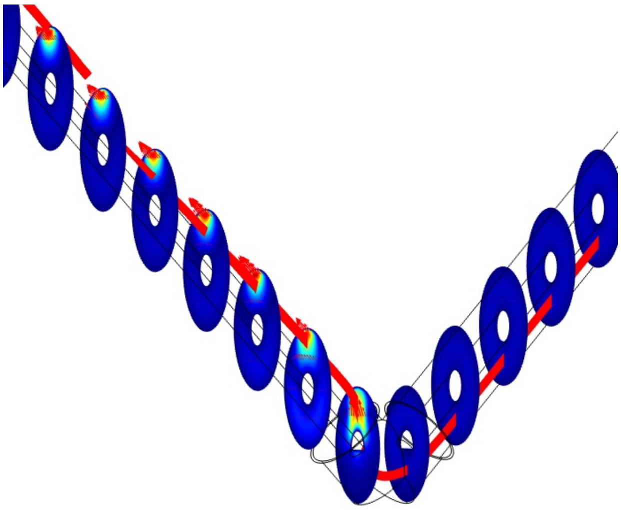

Figure 1: Representative stream lines for liquid phase flow as a result of fluorine gas flux from fluorine cell anode. Gas density indicated using a slice plot.