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Numerical simulation of mass transport in a filter press type electrochemical reactor FM01-LC: Comparison of predicted and experimental mass transfer coefficient

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ABSTRACT

This paper studies flow characteristics and their effect on local mass transfer rate to a flat plate electrode in a FM01-LC electrochemical reactor. 3D reactor simulations under limiting current and turbulent flow conditions were performed using potassium ferro-ferricyanide electrochemical system with sodium sulfate as supporting electrolyte. The model consists of mass-transport equations coupled to hydrodynamic solution obtained from Reynolds-averaged Navier–Stokes equations using standard $k_{-\varepsilon}$ turbulence model, where the average velocity field, the turbulence level given by the eddy kinetic energy and the turbulent viscosity of the hydrodynamic calculation were used to evaluate the convection, turbulent diffusion and the concentration wall function. The turbulent mass diffusivity was evaluated by Kays–Crawford equation using heat and mass transfer analogies, while wall functions, for mass transport, were adapted from Launder–Spalding equations. Simulation results describe main flow properties, concentration profiles throughout the entire volume of the reactor and local diffusion flux over the electrode. Overall mass transfer coefficients estimated by simulation, without fitting parameters, agree closely with experimental coefficients determined from limiting current measurements (1.85% average error) for *Re* between 187 and 1407.

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Keywords: Mathematical modeling; Electrochemical reactors; Hydrodynamics; Mass transfer; Limiting current; Turbulence model

1. Introduction

The FM01-LC reactor is one of the most popular continuousflow electrochemical reactors used for laboratory studies. Its characteristics, advantages, and flexibility of adaptation to different applications have been described in the literature (Walsh, 1993). Even though the patent claims on this design have expired, the FM01-LC continues being a common reference for electrochemical reactors with parallel plates (Frías-Ferrer et al., 2008; Griffiths et al., 2005; Ponce-de-León et al., 2007; Vázquez et al., 2010a,b). Basically, this reactor is made of plates and frames that make up one or several channels for electrolyte circulation. The channel can be filled with electrodes and/or turbulence promoters that modify the flow pattern and produce important changes in reactor performance (Brown et al., 1993; Frías-Ferrer et al., 2008; González-García et al., 2000; Griffiths et al., 2005; Ralph et al., 1996). Other variations to the basic design intended for enhancement of reactor performance have been reported in the literature (Frías-Ferrer et al., 2008; González-García et al., 2000; Oduoza and Wragg, 2002; Ralph et al., 1996; Wragg and Leontaritis, 1997). Many of the previous studies on mass transport in the FM01-LC have been focused mainly on obtaining empirical correlations of dimensionless numbers of the

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