CHEMICAL ENGINEERING RESEARCH AND DESIGN 100 (2015) 422–433

Contents lists available at ScienceDirect

Chemical Engineering Research and Design

journal homepage: www.elsevier.com/locate/cherd

Modeling the effect of non-ideal flow pattern on tertiary current distribution in a filter-press-type electrochemical reactor for copper recovery

Eligio P. Rivero[a,*], *Martín R. Cruz-Díaz*[a], *Francisco J. Almazán-Ruiz*[b], *Ignacio González*[b]

[a] *Departamento de Ingeniería y Tecnología, Universidad Nacional Autónoma de México, Facultad de Estudios Superiores Cuautitlán, Av. 1o de Mayo, Cuautitlán Izcalli 54740, Estado de México, Mexico*

[b] *Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa, San Rafael Atlixco 186, México D.F. 09340, Mexico*

ARTICLE INFO

Article history:
Received 28 September 2014
Received in revised form 29 April 2015
Accepted 30 April 2015
Available online 11 May 2015

Keywords:
Electrochemical reactors
Tertiary current distribution
Turbulent mass transfer
Copper recovery
Butler–Volmer kinetics

ABSTRACT

This work presents the numerical modeling of the effect of hydrodynamics on mass transport and tertiary current and potential distribution in a filter press type electrochemical reactor used to study the copper recovery process. The operating conditions of the reactor were in turbulent regime and under charge and mass transfer mixed control.

For hydrodynamics, the Reynolds averaged Navier–Stokes equations and the standard k–ε turbulence model were used. The mass transfer model was a combination of the convection–diffusion equation and a wall function adapted for mass transfer. The Butler–Volmer kinetics for copper reduction, simplified Tafel equations for water oxidation and ohmic potential drop through the electrolyte were also incorporated into the model. The strategic part of the proposed numerical modeling is the concentration wall function that allows linking the transport equations with Cu^{2+} concentration at the interface in order to obtain, along with interfacial potential, the electrode kinetics. Using this approach it was possible to model a very complex interrelation between physical phenomena and the electrochemical reaction taking place in a reactor under a turbulent flow regime using moderate computer resources. The numerical results obtained are in agreement with experimental data of mass transfer coefficient and current–potential behavior.

1. Introduction

The filter press type FM01-LC electrochemical reactor is a common example of flat plate laboratory scale reactor used to study electrochemical processes, such as synthesis, metal recovery, recycling of industrial effluents, and water treatment. To analyse experimental data from this kind of study it is important to understand the effect of flow pattern on the mass transfer from or toward the electrodes and then on the electrode reaction kinetics and electric potential. The FM01-LC, like other kinds of flat plate electrochemical reactor, exhibits a non-homogeneous flow pattern inside the reactor channel caused by the reactor design, especially the inlet and outlet liquid distributors (Frías-Ferrer et al., 2008; Wragg and Leontaritis, 1997). Stagnant zones, channelling, bypass, recirculation and other observed flow phenomena (Bengoa et al., 2000) give rise to variations in the mass transfer coefficient along the electrodes.

In the FM01-LC reactor for Cu recovery, as in other types of electrochemical reactor, these mass transfer coefficient

---

* *Corresponding author*. Tel.: +52 55 56232071.
E-mail address: priveromtz@msn.com (E.P. Rivero).

http://dx.doi.org/10.1016/j.cherd.2015.04.036

Nomenclature

A	empirical constant
a,b	kinetic constants for water oxidation
B	reactor channel width
C_μ	constant of the turbulence model
$C_{\varepsilon 1}$	constant of the k–ε model
$C_{\varepsilon 2}$	constant of the k–ε model
C^+	dimensionless concentration
C_i	concentration of the electroactive species
$C_{i,0}$	inlet concentration of the electroactive species
$C_{i,w}$	wall concentration of the electroactive species
d_e	equivalent diameter = $2BS/(B+S)$
D_i	diffusion coefficient
D_{iT}	turbulent diffusion coefficient
E	potential
E_a	anodic potential
E_c	cathodic potential
E_{eq}	equilibrium potential of copper reduction
$E_{eq,ox}$	equilibrium potential of water oxidation
E_0	equilibrium cell potential difference
ΔE_Ω	ohmic drop
F	Faraday constant
$\mathbf{F}$	external force
J	current density
J_L	limiting current density
J_a	current density at the anode
J_c	current density at the cathode
$\mathbf{J}$	current density vector
J_0	exchange current density
k	turbulence kinetic energy
k_m	mass transfer coefficient
L	length of the reactor channel
$\mathbf{n}$	vector normal to the wall
$\mathbf{N}_i$	mass transfer flux
$N_{i,w}$	mass transfer flux at the wall
P	pressure
Pc	factor of integration of resistances in near-wall layers
R	gas constant
Re	Reynolds number = $d_e v\rho/\mu$
S	electrode spacing
Sc	Schmidt number = $\mu/(\rho D_i)$
Sc_T	turbulent Schmidt number = $\mu_T/(\rho D_{i,T})$
$Sc_{T\infty}$	constant of the Kays–Crawford model
Sh	Sherwood number = $d_e k_m/D_i$
t	time
T	temperature
$\mathbf{u}$	velocity vector
u	velocity
U	cell potential = $E_a - E_c$
u^+	dimensionless velocity = $u/(\tau_w/\rho)^{1/2}$
V_{in}	inlet velocity
x,y,z	Cartesian coordinates
y^+	dimensionless distance to the wall = $y\rho(\tau_w/\rho)^{1/2}/\mu$
z_i	number of electrons exchanged in electrochemical reaction

Greek letters

α	transfer coefficient
δ^+	dimensionless thickness selected for wall function = $\delta\rho(\tau_w/\rho)^{1/2}/\mu$
ε	turbulent energy dissipation rate
ϕ_a	electrolyte potential at the anode interface
ϕ	electrolyte potential
ϕ_c	electrolyte potential at the cathode interface
κ	Karman constant
μ	viscosity
μ_T	turbulent viscosity
ρ	density
σ	electrolyte conductivity
σ_k	constant of k–ε model
σ_ε	constant of k–ε model
τ	shear stress
τ_w	wall shear stress

variations are very important, not only because of the amount of electroactive species which can reach the electrode surface, but also because of their effect on the overpotential in each zone of the reactor. Mass transfer rate and overpotential are factors involved in the type of metallic copper deposit formed (compactness, grain size, dendrite and powder production) as well as the flow characteristics are involved in the shear stress over the electrode surface for carrying the metallic copper out in the liquid stream. Rough deposit is formed at local laminar hydrodynamic conditions (current electrodeposition lower than the limiting current density conditions), whereas a turbulent local regime provokes dendritric deposits (Bazan and Bisang, 2004; Robinson and Walsh, 1991a, 1991b). In addition, high overpotentials may lead to undesired side reactions that may diminish the charge efficiency of the reactor and lead to uncontrollable changes (pH, conductivity, excessive gas formation, mass transfer rate, formation of solid byproducts, etc.). Therefore, coupling hydrodynamics, mass transport, electrochemical kinetics and potential and current distribution is necessary to obtain a comprehensive understanding of the electrochemical reactor behavior. The importance of the fluid dynamics on mass transport and electrochemical kinetics has been shown by modeling electrodeposition process on rotating electrodes (Mandin et al., 2007a, 2007b, 2006a, 2006b). Also, in processes with intensive gas evolution reactions, as in water electrolysis, there is a strong coupling of these phenomena since the bubble formation diminishes the electrolyte conductivity and modifies the hydrodynamic behavior affecting the current distribution over the electrode (Mandin et al., 2014, 2005). However, modeling tertiary current distribution in an electrochemical process may be very complex, especially for reactors operating under turbulent flow. Thus, several authors have studied the problem using some simplifications: the 2D current distribution over flat plate electrodes and other simple geometries where electrolyte flows in the laminar regimen have been reported (Georgiadou, 2003; Boovaragavan and Basha, 2006). Also, the relationships among mass transfer, ohmic drop and overpotential have been studied for copper electrodeposition in a cell without any type of convection (Pohjoranta et al., 2010). However, very few works have studied electrochemical reactions in reactors under turbulent flow, which is a very important case from a practical point of view. Even though the characteristic lengths of the laboratory scale FM01-LC electrochemical reactor are small, the design of the inlet distributor produces high velocity streams or jets not parallel to reactor walls, which are discharged inside the reactor channel causing 3D flow