Electrochimica Acta 194 (2016) 338–345

Contents lists available at ScienceDirect

Electrochimica Acta

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

Computational fluid dynamic simulations of turbulent flow in a rotating cylinder electrode reactor in continuous mode of operation

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ARTICLE INFO

Article history:
Received 2 December 2015
Received in revised form 12 February 2016
Accepted 13 February 2016
Available online 16 February 2016

Keywords:
Residence time distribution (RTD)
Reynolds averaged Navier–Stokes (RANS) equations
Computational fluid dynamics (CFD)
Rotating cylinder electrode (RCE)

ABSTRACT

Computational fluid dynamics (CFD) simulations were carried out for single-phase flow in a rotating cylinder electrode reactor (RCE) in a continuous operation mode. Velocity profiles and streamlines were obtained solving the Reynolds-averaged Navier-Stokes (RANS) equations with the $k-\varepsilon$ turbulence model. Residence time distribution (RTD) was obtained solving the averaged diffusion-convection equation. Two configurations of RCE, varying the position of the electrolyte flow inlet and flow exit, were tested. Good agreement of simulations with experimental RTD was obtained. A constant rotational speed of 300 rpm (peripheral velocity of 59.7 cm s^{-1}, Re = 22682) at the RCE surface was employed. Velocity profiles, streamlines, and RTD are obtained at different volumetric flow rates ranging from 0.1 to 0.8 L min^{-1}. The flow behavior shows the presence of recirculation zones, being less important for the configuration where the electrolyte inlet is situated at the bottom of the reactor, and the electrolyte outlet is set at the top of the reactor wall surface. The extent of recirculation zones increases with increasing flow rate.

1. Introduction

The rotating cylinder electrode electrochemical reactor (RCE) is one of the most common geometries used in the following studies: metal ion recovery [1–3], alloy formation [1,2], corrosion [1,2], effluent treatment [4–8], and Hull cell studies [9,10]. On the other hand, CFD is often used to describe electrochemical reactor performance, in which the hydrodynamics can be analyzed in detail [11]. Residence time distribution (RTD) has been obtained in different kinds of reactors using CFD, either by the particle tracking method or by the stimulus-response simulation method using different mathematical models [12–14]. Under practical operating conditions, the electrochemical reaction performance is directly related to the reactor hydrodynamics [15].

The flow pattern in a rotating cylinder has been approximated to turbulent flow by Hwang et al. [16,17]. The theoretical approach of this pattern was developed using the Navier-Stokes equations to model the turbulent flow around a rotating cylinder by direct numerical simulation (DNS) in 2D [16]. Moreover, these authors showed that in the fully turbulent layer, there is a logarithmic velocity profile, which is similar to that developed inside tubes and over flat plates [16].

Another approximation employs the RANS equations, which include the turbulent viscosity by means of the standard k-ε turbulence model [8,18,19]. Rivero et al. [8,18] applied a RANS hydrodynamic modeling approach to an RCE in 3D. The theoretical results showed the presence of Taylor vortices around the cylinder surface [18]; we found similar results using four plates as counter electrodes [20].

Enciso et al. [19] studied the hydrodynamic behavior of an RCE solving the RANS-RNG (Renormalization Group) equations in 3D. The authors' simulated results were validated with experimental data obtained by digital image analysis (DIA) on the top of the reactor. Bauer et al. [21] studied multi-ion transport in a RCE, solving the convection–diffusion-migration equations in combination with phenomenological electrode-kinetics modeling in 3D.

Tomasoni et al. [22] characterized the transport phenomena of a RCE using a combination of experimental, numerical, and theoretical approaches. Furthermore, the experimental velocity profiles were obtained with particle image velocimetry (PIV) and compared with velocity profiles theoretically obtained by solving the RANS equations. It is important to highlight that studies on CFD in a continuously operating RCE have so far not been published in the literature. Consequently, there are no studies on the residence time distribution in continuously operating RCE. The CFD simulation of hydrodynamics in a RCE in continuous mode of

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http://dx.doi.org/10.1016/j.electacta.2016.02.076

operation is particularly useful for scaling-up from laboratory to industrial size in applications such as metal ion recovery and wastewater treatment.

In this paper, we model and simulate the RTD of a RCE in a continuous mode of operation. CFD simulations of turbulent flow were performed solving the RANS equations with the $k-\varepsilon$ turbulence model. The turbulent flow was controlled by the RCE rotation speed. RTD was obtained solving the averaged diffusion-convection equation. Two configurations of RCE, varying the position of the electrolyte flow inlet and flow exit were tested. Theoretical RTD were validated with experimental data.

2. Description of the RCE

Fig. 1(a) and (b) show a schematic diagram of two RCE configurations in continuous mode. Configuration one (Fig. 1(a)) consists of a 500 cm^3 acrylic reactor and a 316-type stainless steel cylinder with a diameter of 3.8 cm and a length of 11 cm, as a cathode. Six plates were used as counter electrodes. Each plate was 13 cm long, 2 cm wide and 0.3 cm thick. The electrolyte inlet is located above the acrylic reactor employing a polycarbonate tube with a diameter of 0.4 cm, and the electrolyte outlet is located at the bottom, with a diameter of 1.0 cm. The same RCE was used for configuration two (Fig. 1(b)), but the electrolyte inlet was located at the bottom of the reactor (with a diameter of 1.0 cm), and the electrolyte outlet (with a diameter of 1.0 cm) was located at a height of 10 cm on one side of the top of the reactor. It is important to highlight that during the hydrodynamic experiments in continuous mode, the experimental height of the electrolyte contained in the configuration one and two were 6.7 and 10 cm respectively, which were experimentally conditioned by the position of the electrolyte outlet. Table 1 shows the dimensions of the RCE.

3. Formulation of numerical simulation

The volumetric flow rates studied here were 1.7, 3.3, 5, 6.7 and 13.3 $cm^3 s^{-1}$ (0.1, 0.2, 0.3, 0.4 and 0.8 $L\,min^{-1}$) giving mean flow rates ranging from 0.037 to 0.18 $cm\,s^{-1}$ (performed at the gap area between rotating cylinder and reactor walls). A constant rotational speed of 300 rpm (peripheral velocity of 59.7 $cm\,s^{-1}$, Re = 22682) at the RCE surface was tested here. The peripheral velocity predominates over the inflow electrolyte velocities in the continuous mode. Therefore, the turbulent flow (Re > 100) is imposed by the RCE rotation speed [1].

Like the rotational speed provokes 3D flow instabilities and eddy formation, we solve the RANS and the averaged diffusion-convection equations for the non-ideal flow analysis. For the solution of the RANS equations, we used the standard k-ε turbulent model [18,20]. Two different geometries configurations of the RCE in continuous mode were drawn in the software COMSOL Multiphysics (Fig. 2), using the configurations described in section 2 as a basis for the computational geometry. Fig. 2 also shows the tetrahedral mesh employed in the experiments, which is described in detail below.

3.1. Fluid flow

For an incompressible fluid under turbulent flow the model equations are: Reynolds averaged Navier-Stokes equation (Eq. (1)), where the so-called Reynolds stresses are expressed in terms of the turbulent viscosity (Eq. (2)) and the standard k-ε turbulence model (Eqs. (3) and (4)) [18,20,23,24].

$$(\rho \boldsymbol{u} \cdot \nabla \boldsymbol{u}) = -\nabla P + \nabla \cdot ((\mu + \mu_T)(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)) \quad (1)$$

$$\mu_T = \rho C_\mu \frac{k^2}{\varepsilon} \quad (2)$$

$$\rho(\boldsymbol{u} \cdot \nabla)k = \nabla \cdot \left[\left(\mu + \frac{\mu_T}{\sigma_k}\right)\nabla k\right] + P_k - \rho\varepsilon \quad (3)$$

$$\rho(\boldsymbol{u} \cdot \nabla)\varepsilon = \nabla \cdot \left[\left(\mu + \frac{\mu_T}{\sigma_\varepsilon}\right)\nabla \varepsilon\right] + C_{\varepsilon 1}\frac{\varepsilon}{k}P_k - C_{\varepsilon 2}\rho\frac{\varepsilon^2}{k} \quad (4)$$

where $\boldsymbol{u}$ is the averaged velocity vector, P the pressure, μ the viscosity, μ_T the turbulent viscosity, ρ the density, $C_\mu, \sigma_k, \sigma_\varepsilon, C_{\varepsilon 1}$ and $C_{\varepsilon 2}$ are turbulence model constants, k the turbulent kinetic energy, ε the turbulent energy dissipation rate, and P_k an energy production term ($P_k = \mu_T\left[\nabla \boldsymbol{u} : (\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right]$) [25]. It is important to mention that the notation $()^T$ of Equation (1) denotes the transpose of $\nabla \boldsymbol{u}$, and it should not be confused with any turbulent suffix or quantity such as for example μ_T.

This model is applicable to high Reynolds numbers. For this reason, in the regions close to the wall, where the speed is dependent on the wall, the velocities decrease rapidly and are inaccessible for this model. Wall functions are usually used to solve

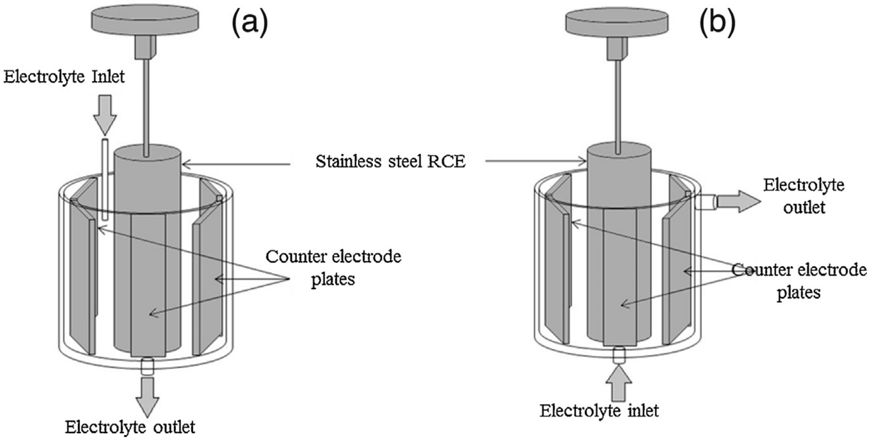

Fig. 1. Continuous rotating cylinder electrode scheme: (a) configuration one, and (b) configuration two.