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Characterization of hydrodynamics and mass transfer in two types of tubular electrochemical reactors

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ABSTRACT

Electrochemical treatment is an environmentally friendly method of removing pollutants from industrial wastewater. The tubular electrochemical reactor is one kind of electrochemical reactor. The current density distribution on the electrode surface in a traditional concentric tubular reactor is not homogeneous and the working area of the anodes and cathodes is unequal. Therefore, a novel tubular electrochemical reactor based on plug flow fluid orthogonal with mesh plate electrodes is presented. In this work, fluid flow and hydrodynamics of the vertical-flow tubular electrochemical reactor, such as velocity distribution and turbulent intensity distribution using computational fluid dynamics (CFD) method, are studied by comparing them to the traditional one. The electro-oxidation of phenol simulation wastewater treatment was developed to analyze the mass transfer performance of the two types of electrochemical reactors. In the novel tubular electrochemical reactor, due to the presence of mesh electrodes, the velocity distribution tended to be more homogeneous. In fact, the turbulent intensity clearly increased by 200% around the electrode surface. The kinetics of organic compounds removal in the novel tubular electrochemical reactor was also improved. Under the same flow rate, the improvement of the mass transfer coefficient for the novel tubular electrochemical reactor was more than twice that of the traditional tubular electrochemical reactor.

1. Introduction

Today's strict environmental laws and regulations have necessitated the need for clean technology in wastewater treatment. Electrochemical reactor systems are of great interest in the wastewater treatment process [1]. Various types of electrochemical reactors are employed in electrochemical applications. These include the box type, filter press type, plate and frame type according to the structure of the electrochemical reactor, or are categorized by batch type, tube type, and continuous mixing chamber according to the working mode.

In the design of electrochemical reactor, the geometrical shape of the electrodes is a key factor because it determines the type of electrolysis cells and is related to easy operation, energy efficiency, economics, and pollutant removal efficiency of electrolysis systems [2–4]. The tubular electrochemical reactor, also named plug flow electrochemical reactor, has a wide range of applications in energy, metallurgy, environmental protection, and other fields [5], and it has attracted great interest because of its various advantages such as improvement in the pollutant removal rate and lower energy consumption [6]. The concentric structure is a classical tubular reactor which has been characterized since the 1970s and has been used to extract gold from electroplating rinse waters and silver from photographic processing liquors [7–9].

In the research literature for the concentric tubular reactor, the rod type of anodes and tube type of cathodes are most popular [10,11]. However, the distribution of current density was not homogeneous due to different surface areas of anodes and cathodes in the reactor, and the coating was unstable and easy to fall off due to different internal stress in electrode materials [12]. In order to solve these problems, we proposed a novel tubular electrochemical reactor with mesh-plate electrode perpendicular to the axial velocity of the fluid in previous work (named vertical-flow tubular electrochemical reactor) [13]. The meshed structure of electrodes provided enough channels for fluid volume orthogonally through electrodes as a plunger flow, and larger acting surfaces for pollutants electrolysis, rather than concentric tubular reactors [14].

Abbreviations: CFD, computational fluid dynamics; CTER, traditional concentric tubular electrochemical reactor; VTER, novel vertical-flow tubular electrochemical reactor.

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Notation

A	anode area, m^2
A_1	single electrode area, m^2
C	constant
c_{org}	organics concentration, mol m^{-3}
d_e	equivalent diameter, m
F	Faraday constant, C mol^{-1}
$\vec{F}$	external force vector, N
I	applied current density, Am^{-2}
I_{lim}	limiting current density for organics electric catalytic oxidation, A m^{-2}
I^0_{lim}	initial limiting current density, A m^{-2}
k_m	mass transfer coefficient, m s^{-1}
l	distance between two electrodes, m
n	total number of electrodes, dimensionless
ΔP	pressure drop of reactor, Pa
ΔP_{exp}	measured pressure drop between inlet and outlet by experiment, Pa
ΔP_1	pressure drop of a single electrode, Pa
ΔP_2	pressure drop between the two electrodes, Pa
S	source of unit volume, dimensionless
S_n	normalised space velocity, m^3 m^{-3} s^{-1}
u	mean velocity of tube, m s^{-1}
u_1	mean velocity of fluid flowing through the electrode, m s^{-1}
V	volume of the electrode,m^3
$\vec{v}$	velocity vector, m s^{-1}
V_R	volume of the reactor, m^3
z	number of electrons, dimensionless

Greek

α	characteristic parameter of the electrolysis process, dimensionless
ε	drag coefficient, dimensionless
μ	dynamic viscosity of fluid, Pa·s
ρ	density, kg m^{-3}
$\vec{\tau}$	stress tensor, N m^{-2}
ϕ	generalized variable, dimensionless
Γ	diffusion coefficient for φ, m^2 s^{-1}

Hydrodynamics of reactors is one of the most important factors determining the kinetic energy consumption, current efficiency, etc., of pollutants removal, and it is required for accurate design and scale-up of reactors. In electrochemical cells, the flow pattern is strongly related to mass transfer and degradation efficiency. Computational fluid dynamics (CFD) is an effective approach to simulating the flow field and optimizing the configuration of reactors because of its advantages such as reduced time and costs [15–17]. By using CFD tools, Ramírez-Muñoz has clarified the fluid behavior in the electrochemical reactor under different operating conditions [18], Martínez-Delgadillo and Mollínedo-Ponce demonstrated that the reactor inlet type had an important influence on reactor performance affecting the back-mixing degree or dispersion [19].

In this work, we analyze velocity distribution, flow pattern, and turbulence intensity of the novel tubular electrochemical reactor with mesh-plate electrode perpendicular to fluid flow by the CFD method and compare the results with that of the concentric tubular reactor. The mass transfer coefficients were obtained associated with tube flow velocity during the treatment of phenol simulation wastewater using both novel and traditional reactors.

2. CFD simulations and experiments

2.1. Geometric models

The vertical-flow tubular electrochemical reactor (VTER) with meshed anodes of Ti/PbO_2 and meshed cathodes of Ti is shown in Fig. 1A. The position of the anode and cathode was alternated with an inter-electrode gap of 20 mm and was perpendicular to the wastewater flow. The holes of electrodes were diamond shaped with a diameter of 50 mm and electrode plate porosity was 0.4, as shown on the right side of Fig. 1A (a, 2 mm and b, 5 mm). As a comparison, a traditional concentric tubular electrochemical reactor (CTER) with a rod anode of Ti/PbO_2 and a tube cathode of Ti with an inter-electrode gap of 20 mm is shown in Fig. 1B. The diameters of the anode and cathode were 9 mm and 49 mm, respectively.

In this research, the total geometric area of anodes (working electrodes) in these two types of reactors was 2.36×10^{-2} m^2. Cylindrical resin casings were also applied and the dimensions and position of the inlet and outlet of both reactors were the same: 500 mm in total length, 50 mm in tube inner diameter, 30 mm in inlet and outlet lengths, 10 mm in inlet and outlet tube diameters. The operating volume was 0.98 L. Tangential manifold was selected for inlet and outlet placement according to previous works [11,13].

2.2. Numerical simulations in CFD

Gambit, a commercial mesh generator, was used to create the grid in this work. An independent analysis of the grid was performed to eliminate errors in simulation accuracy, convergence, numerical stability, and computational steps related to grid coarseness. The computation was carried out with three-dimensional single precision, which produced accurate predictions in all cases. The maximum residual tolerance was 10^{-4} for the continuity equation and momentum equations. The simulation results for different cell numbers were examined, and an optimum grid resolution was established on the condition that the finer mesh did

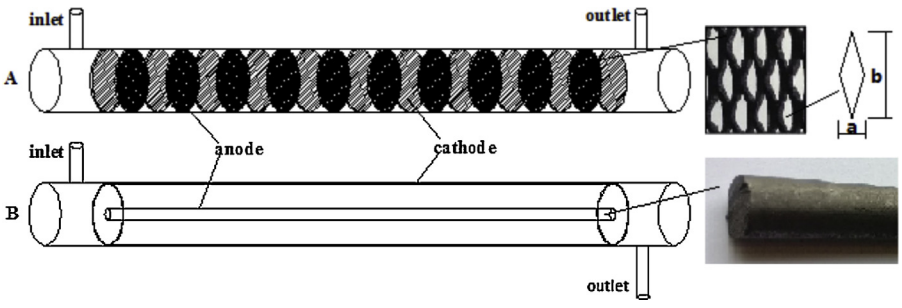

Fig. 1. Schematic diagram of novel vertical (A) and traditional concentric (B) tubular electrochemical reactors.