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Numerical Simulation of the saline water electrolysis process using electromagnetic waves

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ABSTRACT: Microwave irradiation has been used to speed up chemical reactions in comparison to conventional reactions. Because the electromagnetic waves cause increasing molecular vibrations. Energy consumption is reduced by using electromagnetic waves. As a result, electrode corrosion rate is reduced. In this article, a numerical method has been used to compare saline water electrolysis (EL) and saline water electromagnetic electrolysis reactor (EMER). Axisymmetric geometry is considered in simulations and steady and frequency dependent analysis are conducted. Continuity equations and Navier-Stocks equation for fluid flow, and Nernest-Planck equation for mass transfer flow, and the maxwell equation for electromagnetic wave modeling are taken into account. At the first, the effect of electromagnetic waves on the ion separation has been investigated. Results have shown that an obvious enhancement has occurred in ion separation due to electromagnetic irradiation. The dechlorination in EMER process has been improved more than three times in comparison with EL process. Also, the ion separation has been enhanced linearly by increasing the cell potential and initial salinity. The quantitative results of each parameter are shown in the paper.

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1- Introduction

Dechlorination has been defined as a chemical process by which some or most of the chlorine has been removed [1]. Some of problems have been recognized in seawater electrolysis. The main problem is the low conductivity of the electrolyte and subsequent high power requirements [2]. The power consumption comparison of some electrodes and the energy consumption depending on the salinity level for the target oxidants production have been investigated by Lacasa et al. [3]. Also, the influence of salinity, current density and operation mode (batch and single-pass) on inactivation and total residual chlorine production rates have been investigated by Nanayakkara et al. [4]. The microwave-enhanced chemical reactions have presented a dramatic acceleration in reaction rates and selectivity [5]. A wide variety of chemical transformations have been done using a microwave reaction vessel by Zhang and Hayward [6]. The present paper concentrates on the simulation of saline water electrolysis (EL) and saline water electromagnetic electrolysis reactor (EMER) to demonstrate the effect of microwave irradiations on saline water electrolysis.

2- Geometry and computational domain

The geometry and boundary conditions of the present paper are shown in Figure 1. A cylindrical reactor with an outer radius of 18 mm as the cathode, inner radius of 4, 6, 8, and 10 mm as the anode, and the height of 50 mm has been used for the electrolysis process.

3- Chemical Reactions and equations

The electrochemical chlorine evolution reaction and hydrogen evolution reaction are two half-reactions [7]:

$$2Cl^{-}(eq) \rightarrow Cl_2(g) + 2e^{-} \tag{1}$$

$$2H_2O(l) + 2e^{-} \rightarrow 2OH^{-}(eq) + H_2(g) \tag{2}$$

$$2NaCl(eq) + 2H_2O(l) \rightarrow Cl_2(g) + H_2(g) + 2NaOH(eq) \tag{3}$$

The continuity and Navier-Stokes equations have been used for mass and momentum balance. The mass flux of species i in the electrolyte is given by the Nernst-Planck equation. [8]:

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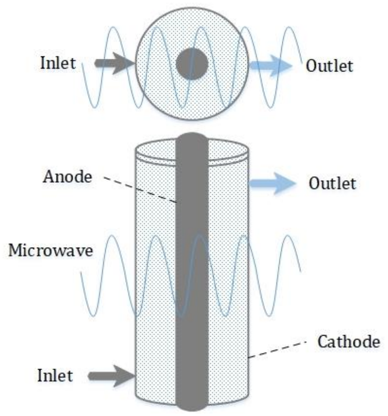

Fig. 1. Schematic diagram of EMER

Table 1. Basic parameters used in the model

Value	Description
10-16 V	DC potential
2.5E−9 m²/s	Diffusion coefficient, Na
2E−9 m²/s	Diffusion coefficient, Cl
298.15 K	Temperature
110-440 mol/m³	Inlet concentration, Na
110-440 mol/m³	Inlet concentration, Cl
0.05 m	Channel length
4-10 mm	Anode Radius
18 mm	Cathode Radius

$$\frac{\partial \rho}{\partial t}+\nabla\left(\rho.\vec{u}\right)=0 \tag{4}$$

$$\frac{\partial \vec{u}}{\partial t}+\rho\left(\vec{u}.\nabla\right)\vec{u}=\nabla p+\nabla\left[\nabla\vec{u}+\left(\nabla\vec{u}\right)^{T}\right]+\vec{F} \tag{5}$$

$$\vec{N_i}=-D_i\nabla c_i-Z_i\mu_i c_i\nabla\Phi+\vec{u}c_i \tag{6}$$

$$\frac{\partial c_i}{\partial t}+\nabla.\vec{N_i}=0 \tag{7}$$

where ρ, u, p, μ, ci, Di, Zi, μi, Φ and u are the density, the velocity vector, the gauge pressure, dynamic viscosity, concentration, diffusion coefficient, charge number of species i, ionic migration, electric potential, and the flow velocity vector respectively. Maxwell's equations and the equation of continuity are a set of equations indicating the relationships between the fundamental electromagnetic quantities [9].

$$\nabla\times\vec{H}=\vec{J}+\frac{\partial\vec{D}}{\partial t} \tag{8}$$

$$\nabla\times\vec{E}=-\frac{\partial\vec{B}}{\partial t} \tag{9}$$

$$\nabla.\vec{D}=\rho \tag{10}$$

$$\nabla.\vec{B}=0 \tag{11}$$

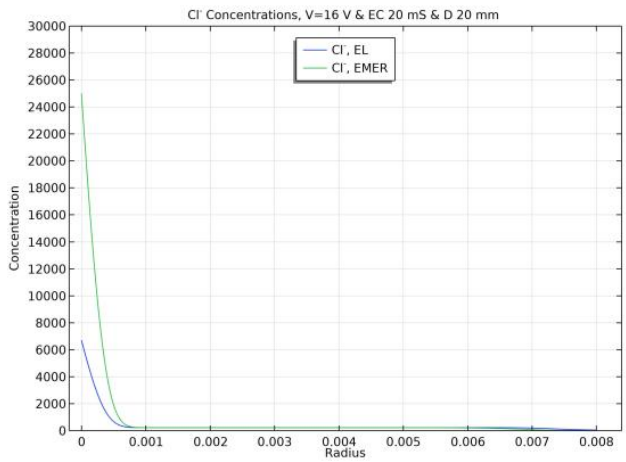

Fig. 2. Comparison of Cl- concentrations (mol/m3) between EL and EMER

$$\nabla.\vec{J}=-\frac{\partial\rho}{\partial t} \tag{12}$$

4- Numerical approach

The COMSOL v6.0 has been used to solve the above-mentioned governing equations. The working conditions including the geometric parameters and other working parameters are listed in Table 1.

5- Results

Figure 2 illustrates the concentration comparison of Cl^- ions between EL and EMER for V=16V and D=20mm. Electromagnetic enhancement in Cl^- ion distributions is

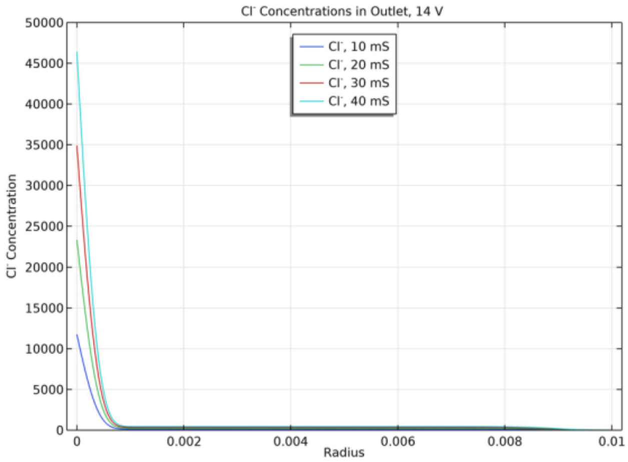

Fig. 3. The effect of salinity on the Cl- concentrations (mol/m3) in EMER

clearly observed. The differences between EMER and EL ion concentrations can be explained by decreasing the energy requirement and increasing the reaction rate in the presence of electromagnetic waves, which illustrates a significant electromagnetic effect.

The effect of salinity on the Cl^- concentration has been shown in Figure 3. It seems that the performance of ion separation has been improved by increasing the salinity.

6- Conclusions

The comparison of EL and EMER have been done numerically and a rapid ion separation increase is observed in EMER simulation because of decreasing the energy requirement under electromagnetic irradiation. Also, As the salinity increased the ion separation raised linearly due to better migration of species in solution.

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