

Numerical Simulation of the saline water electrolysis process using electromagnetic waves

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ABSTRACT

The microwave irradiation has used to speed up chemical reactions in comparison of conventional reactions. Because the electromagnetic waves cause increasing the molecular vibrations. Energy consumption is reduced by using electromagnetic waves. As a results, electrodes corrosion rate is reduces. 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 Nernst-Planck equation for mass transfer flow and maxwell equation for electromagnetic waves modeling are taken into the account. At the first, the effect of electromagnetic waves on the ion separation has been investigated. Results have shown that an obvious enhancement has been occurred in ion separation due to electromagnetic irradiation. The dechlorination in EMER process has been improved more than three times in compare with EL process. Also, the ion separation has been enhanced linearly by increasing the cell potential and initial salinity. Quantitative results of each parameters are shown in the paper.

KEYWORDS

electrolysis, electromagnetic waves, numerical simulation

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1. Introduction

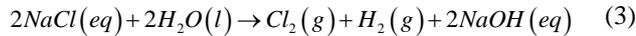
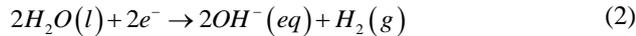
Dechlorination has been defined as a chemical process by which some or most of the chlorine has been removed [1]. Some of problems have been recognized in seawater electrolysis. The main problem is the low conductivity of the electrolyte and subsequent high power requirements [2]. The power consumption 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) in order to demonstrate the effect of microwave irradiations on the saline water electrolysis.

2. Geometry and computational domain

The geometry and boundary conditions of the present paper shown in Figure 1. A cylindrical reactor with the 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 electrolysis process.

3. Chemical Reactions and equations

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



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 Nernst-Planck equation. [8]:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \quad (4)$$

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

$$\vec{N}_i = -D_i \nabla c_i - Z_i \mu_i c_i \nabla \Phi + \vec{u} c_i \quad (6)$$

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \vec{N}_i = 0 \quad (7)$$

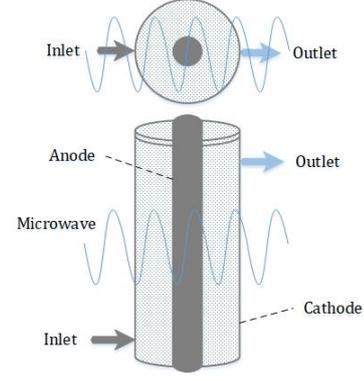


Figure 1. Schematic diagram of EMER

where ρ , u , p , μ , c_i , D_i , Z_i , μ_i , Φ and \vec{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].

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

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \quad (9)$$

$$\nabla \cdot \vec{D} = \rho \quad (10)$$

$$\nabla \cdot \vec{B} = 0 \quad (11)$$

$$\nabla \cdot \vec{J} = -\frac{\partial \rho}{\partial t} \quad (12)$$

4. Numerical approach

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

Table 1. Basic parameters used in the model

Value	Description
10-16 V	DC potential
2.5E-9 m ² /s	Diffusion coefficient, Na
2E-9 m ² /s	Diffusion coefficient, Cl
298.15 K	Temperature
110-440 mol/m ³	Inlet concentration, Na
110-440 mol/m ³	Inlet concentration, Cl
0.05 m	Channel length
4-10 mm	Anode Radius
18 mm	Cathode Radius

5. Results

Figure 2 has illustrated the concentration comparison of Cl^- ions between EL and EMER for $V=16\text{V}$ and $D=20\text{mm}$. Electromagnetic enhancement in Cl^- ion distributions is clearly observed. The differences between EMER and EL ion concentrations can be explained by the decreasing the energy requirement and increasing the reaction rate in the presence of electromagnetic waves, which illustrates a significant electromagnetic effect.

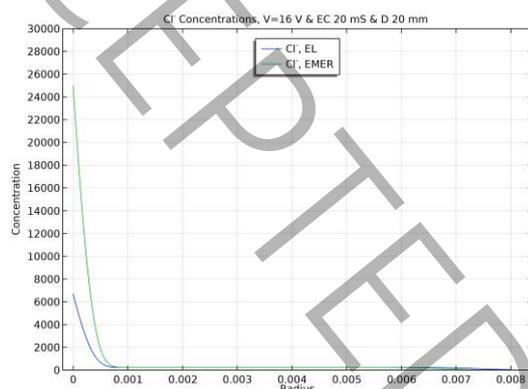


Figure 2. Comparison of Cl^- concentrations (mol/m³) between EL and EMER

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

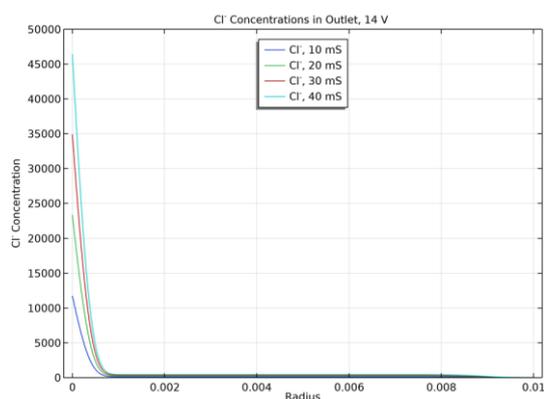


Figure 3. The effect of salinity on the Cl^- concentrations (mol/m³) in EMER

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.

7. References

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