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**Research Paper** 

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Akbar Eghbali\* PhD Candidate

Mohammad Reza Karafi<sup>†</sup> Assistant Professor

Mohammad Hosein Sadeghi<sup>‡</sup> Professor

# Numerical Simulation of the Saline Water Electrolysis Process using Electromagnetic Waves

The electromagnetic waves have been used to accelerate chemical reactions in comparison of conventional reactions. In this article, a numerical method has been used to compare saline water electrolysis (EL) and saline water electromagnetic electrolysis reactor (EMER) in order to realize the effect of electromagnetic waves on electrolysis process. At the first, the effect of electromagnetic waves on the ion separation has been investigated. In the following, influence of main operating parameters such as cell potential (10-16 v), salinity (110-440 mol/m<sup>3</sup> NaCl), electrode diameters (8-20 mm), and microwave frequency (0.3-2.4 GHz) on the ion concentrations have been investigated numerically for an up-flow axisymmetric cylinder. The ion separation in EMER process has been improved dramatically in comparison with EL process. Also, the ion separation has been enhanced linearly by increasing the cell potential and initial salinity.

*Keywords:* Microwave, Desalination, Electrochemical reactor, Energy consumption, Current density, Cell potential

## 1 Introduction

Most of the surface area of the Earth has been covered by seawater, which can be used as a sustainable resource. In order to produce fresh water from seawater, water and energy have been closely interlinked and interdependent valuable resources that underpin economic growth and human prosperity [1, 2]. The energy consumption of desalination processes has highly depended on quality of the source water, the nature of any contamination, and the types of

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<sup>&</sup>lt;sup>\*</sup>PhD Candidate, Faculty of Mechanical Engineering, Tarbiat Modares University, Tehran, Iran, Eghbali.d@gmail.com

<sup>&</sup>lt;sup>†</sup>Corresponding Author, Assistant Professor, Faculty of Mechanical Engineering, Tarbiat Modares University, Tehran, Iran, karafi@modares.ac.ir

<sup>&</sup>lt;sup>‡</sup>Professor, Faculty of Mechanical Engineering, Tarbiat Modares University, Tehran, Iran, sadeghim@modares.ac.ir

process employed [3]. Since the conventional desalination technologies have been operating at very low efficiency, 10–15%, they have not been noble solution for sustainable future water supplies [4]. Production of huge amount of reject brine in desalination processes has been presented and several methods have been used to manage this problem. [5]. The zero liquid discharge (ZLD) as an engineering approach has been introduced to recover a large amount of water from the reject brine, decrease impacts on the planet and achieve sustainability [6]. A series of treatments such as pretreatment have been introduced in ZLD approaches [7].

Seawater electrolysis as a pretreatment in ZLD approach, has been known as a highly potential and widely used in industrial systems and processes [8, 9]. Hsu et al. have studied seawater electrolysis and its chlorine generation efficiency, product quality, and storage stability [10]. Seawater electrolysis have been used in some areas such as marine and offshore industries to produce active chlorine for drinking water and wastewater treatment [11].

Electrolyzed water has been known environmentally friendly with significant disinfection effects [12]. Although many applications of electrolyzed seawater have been reported in aquaculture and seafood processing, few applications have been reported in the agriculture or food processing industries, probably due to sanitary concerns. Plankton and bacteria are abundant in seawater, and certain coastal seawaters suffer from severe contamination [13, 14]. Seawater electrolysis has been attracted much attention in marine and offshore industries over the past few years. Active chlorine has been widely used as one of the oxidants for drinking water and wastewater treatment. The electrolyzed seawater, containing mainly active chlorine species, has attracted extensive attention in marine and offshore industries recently [11]. Lacasa et al. have investigated the power consumption comparison of some electrodes and the energy consumption depending on the salinity level for the target oxidants production [15]. They have shown that the best energy consumption has been received in the same range of current density (30–50 mA/cm<sup>2</sup>) for IrO<sub>2</sub>/Ti and Pt/Ti electrodes. Also, the influence of salinity, current density and operation mode (batch and single-pass) on inactivation and total residual chlorine production rates have been reported by Nanayakkara et al. [16].

The microwave energy has been used to enhance chemical reactions such as organic and peptide synthesis, polymer chemistry, material sciences, nanotechnology, and biochemical processes has been growing at a rapid rate [17]. The saline water has generated dipoles when placed in a microwave field which then has developed orientation polarization, and the lag between the dipole orientation and the electric field leads to heating of the water [18, 19]. In addition, non-thermal effects such as local super heating and generation of nanobubbles have been associated with microwave irradiation [20-22]. Selective interactions of the electromagnetic field with specific substrate molecules, reagents, or catalysts not connected to a macroscopic bulk temperature effect (so-called nonthermal microwave effects) [23, 24]. Also, the microwave process has been known to decrease the activation energy of physical and chemical processes, break down bonded structures and reduce the average particle size salts in aqueous environment [25-28].

A significant microwave selective effects on oxygen inhibition removal have been found for NO decomposition through microwave catalysis over  $BaMn_xMg_xO_3$  catalysts by Xu et al. [29]. Also, they have investigated the effects of a series of reaction parameters, including microwave heating behavior, reaction temperature, outlet gas temperature,  $Mn_2O_3$  loading, microwave input power and  $O_2$  concentration [30]. They have found that the microwave irradiation has exhibited microwave selective effect in the microwave catalytic reaction mode. In addition, they have found that using microwave irradiation to selectively heat the carbon has led to dramatically different observed thermodynamics for the reaction [31]. The highly effective conversion of NO and decomposition of H<sub>2</sub>S via MW catalysis have been investigated by Toukoniitty et al. [32]. They have found that the apparent activation energy (Ea') has decreased substantially under microwave irradiation. Microwave irradiation into advanced oxidation

processes (AOPs) for wastewater treatment has increased the reaction rate of AOPs [33]. Xia et al. have reported that the combination of microwave and oxidants (e.g., H<sub>2</sub>O<sub>2</sub>, PS, PMS) has a synergistic effect and effectively reduces reaction activation energy [34]. The effects of the pyrolysis temperature, heating rate, microwave absorbers, sludge properties and catalysts on microwave pyrolysis (MWP) efficiency and characterization of products have been studied by Li et al. and reducing energy consumption and saving resources have been presented [35].

The chlorine removal rate and energy consumption of microwave-assisted saline water electrolysis were experimentally studied and analyzed by Eghbali et al. [36]. They have observed a rapid energy consumption decrease in the microwave assisted electrolysis process compared to the conventional electrolysis process due to decreasing the activation energy (Ea') under microwave irradiation. An overview of advances in freeze desalination (stand-alone and hybrid) technologies has been provided by Najim [37]. He has reported that the electrical energy consumption and cost of potable water production for this method without latent heat recovery have been less than membrane distillation (MD) and humidification-dehumidification (HDH) methods, similar to the multi effect distillation (MED) and multistage flash distillation (MSF) methods, and higher than the membrane-based desalination method without phase change.

A numerical simulation for electrolytic pickling of stainless steel has been reported by Ipek [38]. Lu et al. [39] have been developed a steady state numerical model for multi-ion parallelplane electrode (PPE) system to investigate the concentration and electric distribution in the process of salt water electrolysis under forced convection. Navier-Stokes and Nernst-Planck equations have been solved using finite element technique to solve this model coupled with ionic diffusion, convection and ionic migration. Numerical studies for spatial evolution of the ionic concentration of an electrolyte in an isothermal electrochemical cell having a porous separator between electrodes have been performed by Borg et al. [40].

Qin and Bau [41] have reported coupled solutions of Nernst-Planck, Navier-Stokes and Maxwell's equations to simulate the MHD (magneto hydrodynamic) flow.

Though there have been several studies on saline water electrolysis, simulation of the electromagnetic electrolysis has not been reported so far. The objective of this work is to numerically investigate whether the performance of the saline water electrolyser can be improved by introducing the electromagnetic waves. Computational approach used in the simulations has been validated with the results reported in an earlier study [39]. Saline water electrolysis (EL) and saline water electromagnetic electrolysis reactor (EMER) have been simulated and compared in present study and the electromagnetic enhancement in results has been observed. Also, the effects of several parameters such as salinity, cell potential, electrode diameter, and frequency of electromagnetic waves have been represented in the saline water electrolysis.

#### 2 Geometry and computational domain

The present study considers the geometry and boundary conditions shown in Figure 1(a). The computational domain has a total of four boundaries (Figure 1(b)). An axisymmetric cylinder has been used as the reactor of electrolysis process. The annular domain has been considered 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. The mass inlet with the several salinities of 110, 220, 330, and 440 mol/m<sup>3</sup> NaCl has been employed on the bottom surface and with specified velocity profile. The outlet boundary has been defined on the top surface of domain. The grid in the near wall regions has been considered to be finer because of the large velocity and concentration gradients in those regions. Also, an imaginary line (cutline) has been considered to calculate the parameters in the middle of channel.



Figure 1(a) Schematic diagram and (b) computational area of microwave assisted electrolysis reactor system

#### **3** Electrode and overall reactions

The electrochemical chlorine evolution reaction (CER) and hydrogen evolution reaction (HER) are two half reactions, which have been occurred at the anode and cathode electrodes of saline water electrolysis, respectively [42].

These reactions have been written as following:

$$2Cl^{-}(aq) \rightarrow Cl_{2}(g) + 2e^{-}$$
(1)

$$2H_2O(l) + 2e^- \rightarrow 2OH^-(aq) + H_2(g)$$
 (2)

$$2 \operatorname{NaCl} (aq) + 2H_2O (l) \to Cl_2 (g) + H_2 (g) + 2 \operatorname{NaOH} (aq)$$
(3)

Two harmful reactions often occur in saline water electrolysis process are generating hypochlorous acid (HOCl) at pH less than 7.46 (Equation (5)) and hypochlorite ions (ClO<sup>-</sup>) at pH more than 7.46 (Equation (6)) [43].

$$Cl^- + 2H_2O \rightarrow HOCl + H^+ + 2e^-$$
(5)

$$Cl^- + 20H^- \rightarrow Cl0^- + H_20 + 2e^-$$
 (6)

Na<sup>+</sup>, Cl<sup>-</sup> and OH<sup>-</sup> are the ions carrying currents.

#### **4** Mathematical equations

The saline water has been assumed as an incompressible Newtonian fluid and the fluid flow under the prescribed inlet velocity has been supposed laminar. The applicable Navier-Stokes equations for continuity and momentum balance have been presented as follow:

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (\partial . \vec{u}) = 0 \tag{7}$$

$$\frac{\partial \vec{u}}{\partial t} = \partial(\vec{u}.\nabla)\vec{u} = \nabla \mathbf{p} + \nabla[\mu(\nabla \vec{u} + (\nabla \vec{u})^T)] + \vec{F}$$
(8)

where  $\rho$ , u, p and  $\mu$  are the density, the velocity vector, the gauge pressure, and the dynamic viscosity, respectively. When an ionic solution has been subjected to an electric field, transport of species has been occurred by three mechanisms: (1) migration (because of potential gradient), (2) convection (because of bulk flow) and (3) diffusion (because of concentration gradient). Migration has implied that negative ions migrate from a negative potential to a positive potential along the opposite direction of the electric field and vice versa for positive ions [44]. Convection does not contribute to the electric currents because of the constraint condition of electroneutrality. Therefore, the electric current is only transported by diffusion and migration of each ionic species. The mass flux of species i in the electrolyte is given by Nernst-Planck equation [39]:

$$\overline{N_i} = -D_i \nabla c_i - Z_i \mu_i c_i \nabla \Phi + \vec{u} c_i \tag{9}$$

where  $c_i$ ,  $D_i$ ,  $Z_i$ ,  $\mu_i$  ( $\mu_i = D_i F/RT$  Nernst–Einstein equation, where F is the Faraday constant, R is the gas constant, T is the thermodynamic temperature),  $\Phi$  and u are concentration, diffusion coefficient, charge number of species i, ionic migration, electric potential, and the flow velocity vector respectively. Also, the equation for mass conservation of species i is the following [39]:

$$\frac{\partial c_i}{\partial t} + \nabla . \overrightarrow{N_i} = 0 \tag{10}$$

Maxwell's equations are a set of equations indicating the relationships between the fundamental electromagnetic quantities [45]. For general time-varying fields, Maxwell's equations can be written as following [45]:

$$\nabla \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t} \tag{11}$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \tag{12}$$

$$\nabla . \vec{D} = r \tag{13}$$

$$\nabla . \vec{B} = 0 \tag{14}$$

where E, D, H, B, J and r are the electric field intensity, the electric displacement or electric flux density, the magnetic field intensity, the magnetic flux density, the current density and the electric charge density, respectively. The first two equations (11 and 12) are also referred to as Maxwell-Ampere's law and Faraday's law, respectively. Equation 13 and 14 are two forms of Gauss' law in the electric and magnetic fields, respectively. The equation of continuity is another fundamental equation, which can be written as following [43]:

$$\nabla . \vec{J} = -\frac{\partial r}{\partial t} \tag{15}$$

#### **5** Summary of numerical approach

In this simulation, COMSOL v6.0 has been used to solve the above-mentioned governing equations with specified boundary conditions. The working conditions included the geometric parameters and other working parameters are listed in Table (1). The electromagnetic wave has been simulated to improve the saline water electrolysis process with the frequencies of 0.45-2.4 MHz.

The migrative and diffusive charge and species transport in the electrolyte are modelled using the Nernst–Planck equations, assuming electroneutrality. The electrochemical model uses the Tertiary Current Distribution, Nernst-Planck interface to predict the transport and reaction in the saline water electrolysis. Charge transport is assumed to take place radially to and from the electrodes. The Frequency Domain interface has been used to solve the Electromagnetic and it assumes that all variations in time occur as sinusoidal signals. Also, it is assumed that all material properties used to solve Maxwell's equations are constant over a single period of oscillation of the electromagnetic wave.

Value	Description
10-16 V	DC potential
$2.5E-9 \text{ m}^2/\text{s}$	Diffusion coefficient, Na
$2E-9 \text{ m}^2/\text{s}$	Diffusion coefficient, Cl
298.15 K	Temperature
110-440 mol/m <sup>3</sup>	Inlet concentration, Na
110-440 mol/m <sup>3</sup>	Inlet concentration, Cl
0.05 m	Channel length
4-10 mm	Anode Radius
18 mm	Cathode Radius
0.45-2.4 GHz	Frequency

Table 1 Basic parameters used in the model

In order to verify the accuracy of the simulation results, the calculated fluid velocity in the channel has been compared with the analytical solution of Abbasov et al. [46]. As shown in Figure (2), it is obvious that the present numerical results have been in good agreement with the analytical solutions. Therefore, the analytical profile has been introduced as inlet velocity profile to simplify the model simulation. 2D and 3D velocity contour of the saline water electrolysis reactor for electrode diameter of 20 and 8 mm have been illustrated in Figure (3).



Figure 2 Comparison between the numerical and analytical results of the axial velocity in the channel





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Figure 3 2D and 3D velocity contour of the saline water electrolysis reactor with (a) 20 and (b) 8 mm electrode diameter

#### 6 Results and discussion

6.1 Evaluation of grid size independence









Figure 5 The (a) Cl- and (b) Na+ concentrations at the EMER outlet and several grid sizes

Grid	Nv * Nr	Grid Number	Cl- separation	Deviation from
0114	1,1,1,1,1,1		(%)	reference grid, III (%)
Mesh I	90 * 60	5400	32.3	13.64
Mesh II	120 * 80	9600	36.4	2.67
Mesh III	150 * 100	15000	37.4	-
Mesh IV	225 * 150	33750	37.7	0.80

In order to ensure the mesh size independence of the present simulations, four typical different grid sizes demonstrated in Figure (4) (i.e., grids I to IV representing 5,400, 9,600, 15,000 and 33,750 cells, respectively) are examined at the cell potential of 14 V, initial salinity of 20 mS and anode diameter of 16 mm. From Figure (5) displaying the ion concentrations at the EMER outlet and several grid sizes and also from Table (2), it can be observed that mesh III with 15,000 cells produces minor percentages of deviations concerning the results on ion separation as compared with mesh IV (i.e., the finest mesh). Therefore, grid III is chosen throughout the present work.

#### 6.2 Verification of Present Simulations

In order to verify the relative accuracy of the present results, direct comparisons of Clconcentrations with the author's experimental data [36] are made at four various anode diameters, as depicted in Figure (6). The experimental setup has employed the same geometry with Al and Fe metal as anodes. As represented in Table (3), the present results demonstrate reasonable agreement with the experiments, giving deviations of approximately 5.94% and 5.21% on average with experimental results with Al and Fe anode, respectively.



Figure 6 The Cl- concentrations at the EMER outlet: Comparison of present model with experimental data [36]

D [mm]	Experimental Cl- concentrations, Al [%]	Experimental Cl- concentrations, Fe [%]	Numerical concentrations [%]	Deviation from experiment, Al (%)	Deviation from experiment, Fe (%)
8	40.5	43.3	43.1	6.26	0.45
12	38.3	40.5	38.0	0.68	6.17
16	35.1	40.3	37.4	6.56	7.25
20	36.3	43.0	40.0	10.26	6.95

 Table 3 The Cl- concentration predictions by model as compared with experiment [36]

The rate of chemical processes, or what may loosely be termed the speed of reaction, can be influenced by changing the concentrations of reactants. Also, the rate of electrochemical processes also can be manipulated by changing the electrode potential. In addition, the rate of an electrochemical reaction can best be described as the electric current density.

#### 6.3 Influence of electromagnetic wave

The concentration comparison of Cl<sup>-</sup> and Na<sup>+</sup> ions between EL and EMER for V=16V and D=20mm have been depicted in Figure (7). The Anode and cathode electrodes have been corresponded to the left side and right side of diagrams, respectively and the horizontal axis of diagrams has been corresponded to anode to cathode distance. It seems that Cl<sup>-</sup> and Na<sup>+</sup> ions have been inclined to anode and cathode electrodes, respectively. Electromagnetic enhancement in 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. The microwave irradiation has exerted nonthermal effects through interaction between electric fields and specific polar molecules. The microwave nonthermal effects can reduce the resistance of ions by rotating dipolar water molecules.

These nonthermal effects have changed the mobility of molecules to move easier and more through electric field. This phenomenon has caused to more ion separation in EMER process in comparison with EL process.



Figure 7 Comparison of (a) Cl<sup>-</sup> and (b) Na<sup>+</sup> concentrations (mol/m<sup>3</sup>) between EL and EMER (V=16V, D=20mm)

In order to verify the ion separation along the channel, the Cl<sup>-</sup> and Na<sup>+</sup> concentrations for EL and EMER and in outlet and cutline (middle of channel) have been shown in Figure (8). These results have depicted that more than 75% of ion separation in outlet has been done until cutline for all cases.





Figure 8 Comparison of  $Cl^-$  and  $Na^+$  concentrations (mol/m<sup>3</sup>) between cutline and outlet for (a) EL and (b) EMER (V=16V, D=20mm)

## 6.4 Influence of anode diameter

By increasing anode diameter from 8 to 20 mm, anode and cathode distance decrease from 14 to 8 mm and the effective area of anode increase. The space between two electrodes also affects the reactions in the electrolysis reactor. During electrolysis, the solution close to the cathode becomes more concentrated because of the different mobilities of the ions present, and this effect can be reduced by agitation of the bulk solution. The gap between electrodes gets partially filled with products during electrolysis, which increases its electrical resistance. Figure (9) has illustrated the  $Cl^-$  and  $Na^+$  concentrations at four different electrode diameters and EL process. In the conventional electrolysis process, as diameter is increased (or as anode to cathode distance is decreased) the ion separation is decreased due to increasing of electrolyte resistance and instability of ion separation. The anode to cathode distance has significant effect on the performance and the efficiency of the electrolysis cell. Lower removal efficiencies of the ion separation in the lower distance between the electrodes would be based on this fact that the power dissipations could be increased in lower anode to cathode distance and higher anode diameter. Also, the mobility of ions has been declined while anode to cathode distance decreased.

Also, 3D molar concentration contours along the four different electrode diameters of EL process and for Cl<sup>-</sup> and Na<sup>+</sup> have been shown in Figures (10) and (11), respectively. It can be seen that by moving the solution from inlet to outlet, the mole concentration near the electrodes increased. In addition, when the distance from electrode increased, the molar concentration dropped evidently. It would be because of electric field distribution between the electrodes. Electric field has been decayed exponentially with increasing distance from the electrodes. Therefore, the electric field would be stronger near the electrodes and positive and negative ions have been gathered in the near region of cathode and anode electrodes, respectively. Moreover, it is obvious that the most part of ion separation has been done until cutline.





Figure 9 The (a) Cl<sup>-</sup> and (b) Na<sup>+</sup> concentrations at the EL outlet and several electrode diameters



Na<sup>+</sup> Concentrations in Outlet, 14 V & EC 20 mS





Figure 10 3D Cl<sup>-</sup> concentration contours along the EL channel and the electrode diameter of (a) 8, (b) 12, (c) 16, and (d) 20 mm







Figure 11 3D Na<sup>+</sup> concentration contours along the EL channel and the electrode diameter of (a) 8, (b) 12, (c) 16, and (d) 20 mm

The Cl<sup>-</sup> and Na<sup>+</sup> concentrations at four different electrode diameters and EMER process have been depicted in Figure (12). In the conventional electrolysis process as diameter is increased (or as anode to cathode distance is decreased) the ion separation is decreased. However, the results of EMER simulation indicate that increasing anode diameter would decrease ion separation but not beyond a value.

It appears in Figure (9) that the minimum ion separation at the electrode diameter of 16 mm according to anode and cathode distance of 10 mm. Decreasing the ion concentration while the electrode diameter increased from 8 to 16 mm is attributed to the increasing of electrolyte resistance and instability of ion separation. In addition, this result can be explained by the fact that, the anode to cathode distance should be just sufficient to provide sufficient turbulence in between the electrodes that initiates mass transfer within the reactor. On the other hand, the higher ion concentration at anode diameter of 20 mm could be due to decreasing in mass transfer and the movement of participant species, leading to the decline of the reaction rate.

In here, it is appropriate to restrict the anode to cathode distance, since the saline water electrolysis may require frequent polarity reversal because of the frequent mass transfers induced by the lower level of turbulence in between the electrodes. In addition, since the ohmic potential drop is proportional to the anode to cathode distance, reducing this gap is of great importance in reducing the electrolysis energy consumption and improving the ion separation.



Figure 12 The (a) Cl<sup>-</sup> and (b) Na<sup>+</sup> concentrations at the EMER outlet and several electrode diameters

In addition, Figures (13) and (14) have demonstrated the 3D molar concentration contours along the four different electrode diameters of EMER process and for  $Cl^-$  and  $Na^+$ , respectively. It is obvious that because of a very high electric field near the electrodes, the mole concentration has been increased by getting close to the electrodes.





Figure 13 3D Cl<sup>-</sup> concentration contours along the EMER channel and the electrode diameter of (a) 8, (b) 12, (c) 16, and (d) 20 mm





Figure 14 3D Na<sup>+</sup> concentration contours along the EMER channel and the electrode diameter of (a) 8, (b) 12, (c) 16, and (d) 20 mm



Figure 15 The influence of anode diameter on the outlet Cl- concentration in the EL and EMER processes

The effect of anode diameter on the molar concentration of Cl<sup>-</sup> at the outlet is illustrated in figure 15 for both EL and EMER processes. Also, the percentage of Cl<sup>-</sup> separation is written in the figure. The maximum and minimum molar concentrations in EMER process equals 94.7 and 82.2 mol/m3 for anode diameters of 8 and 16 mm, respectively. A rapid Cl<sup>-</sup> separation increase has been observed in the EMER process compared to the EL process that could be due to the interactions between electromagnetic waves and molecules in chemical reaction systems. The ratio between EMER and EL processes Cl<sup>-</sup> concentration has been obtained in the range of 3.17-3.74 for all anode diameters. The maximum and minimum Cl<sup>-</sup> separation improvement have been occurred for anode diameter of 20 and 12 mm, respectively.

#### 6.5 Influence of cell potential

The potential difference is caused by the ability of electrons to flow from one half cell to the other. The cell potential has determined the direction of electron flow and the efficiency of the overall cell reaction. The migration of species in the ionic solution has been influenced directly by cell potential. Therefore, cell potential strongly influences both ion separation and mass transfer at the electrodes based on the quantity of electricity that passed through the electrolytic solution. As cell potential increased, the migration of species in solution increased. Figure (16) displays the molar concentration at different cell potential. As expected, the ion separation enhanced as cell potential increased. When higher cell potential has been applied to the electrodes, more positive ions move to the cathode while more negative ions move to the anode. At higher cell potential, an accumulation of ions is caused by the increased electron transfer. The amount of ion separated or collected near the electrodes is dependent on the quantity of electricity that passed through the electrolytic solution. At high cell potential, the extent of electron transfer increases, which results in an increase in the ion separation. It means that performance of ion separation has been improved by increasing the cell potential.



Figure 16 The (a) Cl<sup>-</sup> and (b) Na<sup>+</sup> concentrations at the EMER outlet and several cell potentials



Figure 17 The influence of cell potential on the outlet Cl<sup>-</sup> concentration in the EL and EMER processes

Figure (17) depicts the influence of cell potential on the molar concentration of Cl<sup>-</sup> and percentage of Cl<sup>-</sup> separated at the outlet for EMER process. The results have shown that the Cl<sup>-</sup> concentration and Cl<sup>-</sup> separation increase linearly with increasing cell potential. The Cl<sup>-</sup> concentration has increased from 55.66 mol/m<sup>3</sup> (corresponding to 25.3% Cl<sup>-</sup> separation) for cell potential of 10 V to 95.70 mol/m<sup>3</sup> (corresponding to 43.5% Cl<sup>-</sup> separation) for cell potential of 16 V.

#### 6.6 Influence of salinity

The salinity (and/or conductivity) is an important parameter to optimize electrochemical processes. It is expected that by increasing the conductivity, the saline water electrolysis has been improved. Figure (18) illustrates the molar concentrations of Cl<sup>-</sup> and Na<sup>+</sup> at several inlet salinities. It is obvious that the solution conductivity (EC) increases as the salinity increased. Figure 18 depicts that as salinity is increased the molar separation is increased because of raising reaction rates due to increasing the solution conductivity.

This result can be potentially explained by the fact that, when the initial salinity (conductivity) were higher, less electron transfer (and less current density and energy) were needed to separate ions. The 40 mS electric conductivity (corresponding to 40 PSU salinity) has been found the best value for achieving higher ion separation.

The influence of initial salinity on the molar concentration of Cl<sup>-</sup> and percentage of Cl<sup>-</sup> separated at the outlet is demonstrated in Figure (19) for EMER process. It seems that as initial salinity increases, the Cl<sup>-</sup> concentration and dichlorination are increased. The value of Cl- concentration enhances from 41.3 to 163.4 mol/m<sup>3</sup>, while the initial salinity increases from 10 to 40 mS. In addition, the percentage of dichlorination has remained relatively stable for all salinities.



Figure 18 The (a) Cl<sup>-</sup> and (b) Na<sup>+</sup> concentrations at the EMER outlet and several salinities











Figure 20 The (a) Cl<sup>-</sup> and (b) Na<sup>+</sup> concentrations at the EMER outlet and several frequencies

Microwave is a form of electromagnetic wave in the frequency range 300 MHz (i.e., 0.3 GHz) to 300 GHz, with corresponding wavelengths of 1 mm to 1 m. The EMER process has been simulated in eight microwave frequencies (300 MHz, 450 MHz, 700 MHz, 900 MHz, 1.1 GHz, 1.4 GHz, 1.8 GHz, and 2.4 GHz) to demonstrate the effect of frequency on EMER process. Figure (20) illustrates the molar concentrations of  $CI^-$  and  $Na^+$  at several frequencies of electromagnetic wave. As seen, the ion separation slightly decreased as microwave frequency increased. When the frequency range of the oscillations has been in appropriate range, adequate inter-particle interaction would be enabled. At the high frequency range of the oscillations, inter-molecular forces have tried to stop the motion of a polar molecule before it tried to follow the field. On the other hand, the polar molecule has gotten sufficient time at the low frequency range of the oscillations have been occurred between the adjoining particles in the lower frequencies.

Although the presence of electromagnetic wave has an impressive effect on ion separation, the frequency of microwave in the range of 300 MHz to 2.4 GHz has not a significant influence on the performance of saline water electromagnetic electrolysis. Since the microwave radiation has the appropriate frequency to oscillate polar particles and enable enough interparticle interaction, the ion separation changes versus frequency in the microwave range are so limited. Figure (21) displays the effect of frequency on the molar concentration of Cl<sup>-</sup> and percentage of Cl<sup>-</sup> separated at the outlet for EMER process. The Cl<sup>-</sup> concentration has slightly decreased from 85.6 mol/m3 (corresponding to 38.9% Cl<sup>-</sup> separation) for frequency of 300 MHz to 77.6 mol/m3 (corresponding to 35.3% Cl<sup>-</sup> separation) for frequency of 2.4 GHz.



Figure 21 The influence of electromagnetic wave frequency on the outlet Cl<sup>-</sup> concentration in the EL and EMER processes

## 7 Conclusion

(1) In this paper a numerical method based on the finite element is developed and comparison of saline water electrolysis (EL) and saline water electromagnetic electrolysis reactors (EMER) have been done numerically. The effect of parameters such as cell potential, salinity, electrode diameter and frequency on the ion concentration have been studied.

(2) A rapid ion separation increase is observed in EMER simulation in comparison with EL because of decreasing the energy requirement under electromagnetic irradiation. The ion separation ratio between EMER and EL processes was calculated in the range of 3.17-3.74.

(3) In the EL model as anode to cathode distance is decreased (correspond to higher anode diameter), the ion separation is decreased. The results show that the maximum ion separation is observed at the anode diameter of 8 mm for both EL and EMER models. However, the anode diameter correspond to the minimum ion separation is 20 and 16 mm for EL and EMER models, respectively.

(4) As the cell potential increased the ion separation raised linearly due to better migration of species in solution. The best  $Cl^{-}$  separation was obtained 43.5% for cell potential of 16 V.

(5) Optimum salinity corresponding to maximum ion separation is equal to 40 mS. However, the percentage of Cl<sup>-</sup> separation was remained relatively stable, while the initial salinity was increased.

(6) As the microwave frequency decreased, the EMER performance enhanced slightly. The frequency in the range of 300 MHz to 2.4 GHz has not a considerable effect on the Cl<sup>-</sup> separation.

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## Nomenclature

English symbols

В	Magnetic flux density
Сі	Concentration of species i
D	Electric displacement or electric flux density
$D_i$	Diffusion coefficient of species i
Ε	Electric field intensity
ЕС	Electrical conductivity
EL	Saline water electrolysis
EMER	Saline water electromagnetic electrolysis reactor
F	Faraday constant
Η	Magnetic field intensity
J	Current density
Nr	Grid number in radial direction
Ny	Grid number in axial direction
p	Gauge pressure
r	Electric charge density
R	Gas constant
R_a	Anode diameter
R_c	Cathode diameter
t	Time
Т	Thermodynamic temperature
u	Velocity vector
V	Cell potential
Vel	Axial velocity
$Z_i$	Charge number of species i
Greek symbols	

- $\rho$  Density
- $\mu$  Dynamic viscosity
- $\mu_i$  Ionic migration of species i
- $\phi$  Electric potential