Amirkabir Journal of Mechanical Engineering

Amirkabir J. Mech. Eng., 53(11) (2022) 1401-1404
DOI: 10.22060/mej.2021.19769.7104

Simulation of Effective Parameters on Desalination Water Using Capacitive Deionization Method

A. Abolghasemi, S. Seddighi*

Department of Mechanical Engineering, K. N. Toosi University of Technology, Tehran, Iran

ABSTRACT: Capacitive deionization is one of the membrane methods available for water desalination that works based on ion exchange. In capacitive ionization systems, saline water passes through a cell that has electrodes with a high contact surface. By applying a voltage, the ions are absorbed under an electric field on the surface of the porous electrodes, as a result of which the salinity of the water is reduced and freshwater is removed from the other side of the system. Recently, researchers have proposed various models for predicting the behavior of desalination plants by capacitive deionization. The model used for the simulation is a one-dimensional transfer equation based on the transfer theory of porous and ball-Chapman-Stern electrodes to predict the output water concentration and identify the parameters affecting the performance of the capacitive deionization system. This study aimed to investigate the water desalination efficiency using changes in the operating parameters of capacitive deionization systems. The parameters studied in this study included fluid flow, applied electric current, input concentration, porosity, electrode cross-section, and electrode length. The results showed that the most effective parameter in improving the performance of the device is applied electric current so that with a fifty percent increase in applied electric current, the percentage of water desalination increased by about 72%, and the time required to achieve maximum water desalination decreased by about 76%.

Review History:

Received: Mar. 19, 2021
Revised: May, 31, 2021
Accepted: Jun. 19, 2021
Available Online: Jul. 17, 2021

Keywords:

Capacitive deionization
Ion exchange membrane
Flow-through configuration
Water desalination
Numerical simulation

1- Introduction

Capacitive deionization uses an electrochemical method for separating salt from aqueous solutions producing sweet water by utilizing the absorption of excess ions when the electrodes are charged by an external power supply [1]. The capacitive deionization is performed in a cycle consisting of two stages: the first stage being the electrical absorption of ions or the charge of purification of water in which the ions are immobilized and stopped at the pair of porous carbon electrodes. The next step is the release of ions from the electrodes, where takes place and the electrodes' desorption are regenerated [2]. Suss et al. [3] introduced the method of current flow through the electrode, in which direct current passes through the electrodes. Using the theory of macroscopic porous electrodes, they showed that the Flow-through configuration method would be able to significantly reduce the desalination time and could desalinate water with higher salinity.

In capacitive deionization, water is desalinated by storing ions in electrical dual layers in carbon pores. Biesheuvel et al. [4] proposed a dynamic method involving a constant electric charge in the pores and showed this model can predict different laboratory observations. Their method also predicted some high-salt operating regimes.

Jande and Kim [5] developed a mathematical model of transient absorption to predict the minimum effluent concentration and charge time in the cell at constant voltage, using the charge and current variables, such as potential use, fluid flow, and electrode capacity. In subsequent studies, Jande and Kim [6] proposed a short response model to describe the changes in effluent concentration over time in the constant flow mode of colleagues. Yatian Qu et al. [7] proposed a model for describing the desalination performance of the Flow-through configuration system by focusing on understanding and characterizing the effects of mass absorption and transfer coupling. Their work is the first model that can be used to predict the concentration of output in the water system of capacitive sweeteners by considering the interaction of mass transfer, electric charge, and velocity.

2- Methodology

Eq. (1) represents the general form of the one-dimensional transfer equation for the simulation of the ion deionization cell, of which Fig. 1 is an overview, based on the Gouy-Chapman-Stern transfer electrode theory [7].

$$\frac{\partial c_e}{\partial t}+\frac{2Q}{P_M V_0}\left(c_e-c_0\right)=-\frac{2\lambda I_0}{P_M V_0 F} \tag{1}$$

*Corresponding author's email: Sadegh.seddighi@kntu.ac.ir

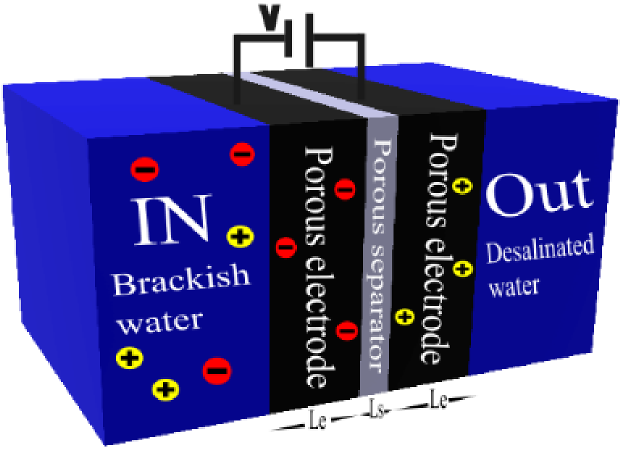

Fig. 1. Schematic diagram of capacitive deionization cell

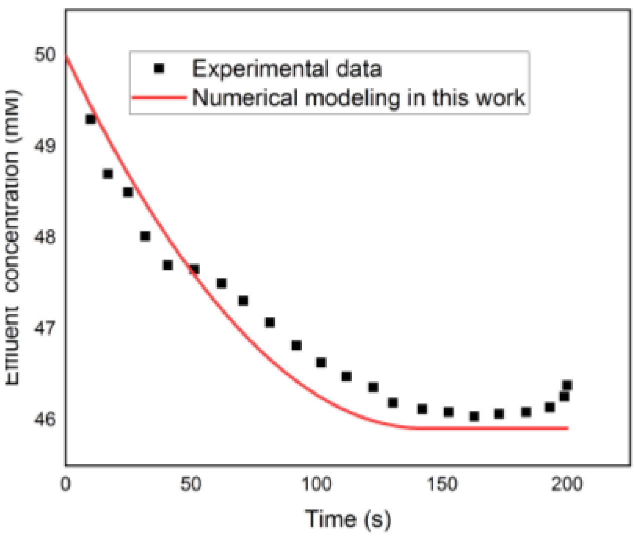

Fig. 2. Comparison of the Experiment [7] and numerical results based on the data in Table 1

The value can be obtained from Eq. (2)

$$\lambda \approx \frac{I_0 t}{8 P_m V_e c_0 F} \quad (2)$$

Eqs. (3) and (4) is the response of Eq. (1) to the values and will be as follows

$$c_e(t) = c_0 - \left(\frac{B}{A^2}\right)\left(1 - e^{-At}\right) + \left(\frac{A}{B}\right)t \quad (3)$$

$$c_e(t) = \left(\frac{C}{A}\right) + K_1\left(e^{-At}\right) + c_0 \quad (4)$$

Where the values of the parameters A and B and C are obtained from Eq. (5) below.

$$A = \frac{2Q}{P_M V_0}, \quad B = -\frac{I_0^2}{4 P_M P_m V_0 V_e c_0 F^2}$$
$$C = -\frac{2 I_0}{P_M V_0 F} \quad (5)$$

The percentage of changes in the concentration of the effluent water concentration is defined as Eq. (6).

$$\%C = \frac{C_o - C_i}{C_o} \times 100 \quad (6)$$

3- Results and Discussion

Fig. 1 shows a schematic diagram of a capacitive deionization cell. The electrode material used in the laboratory model is a hyperical integrated carbon airgel. To confirm the results obtained from numerical solutions, these results must be validated. In this study, the results of the numerical solution have been validated by laboratory research conducted by Yatian Qu et al. This is a validation for the values given in Table 1. The process of the graph obtained from the results shows good coordination with the laboratory data, the results of which can be seen in Fig. 2.

This study aims to investigate the efficiency of water desalination using changes in system operating parameters. The parameters studied in this study include fluid flow, applied electric current, input concentration, porosity, electrode cross-section, and electrode length. Figs. 3 to 8 shows the concentration of output water with changes in system operating parameters.

Table 1. Parameter values used in this work

Parameter	description	value	unit
P_M	macropore porosity	0.57	
P_m	micropore porosity	0.1	
V_0	entire cell volume	1.57	cm^3
L_e	thickness of electrode	300	μm
L_s	thickness of separator	100	μm
V_e	volume of electrode	1.3	cm^3
c_0	feed salt concentration	50	mM
I_0	charging current	50	mA
F	Faraday constant	96485	sA/mol
Q	flow rate	7.7	ml/min

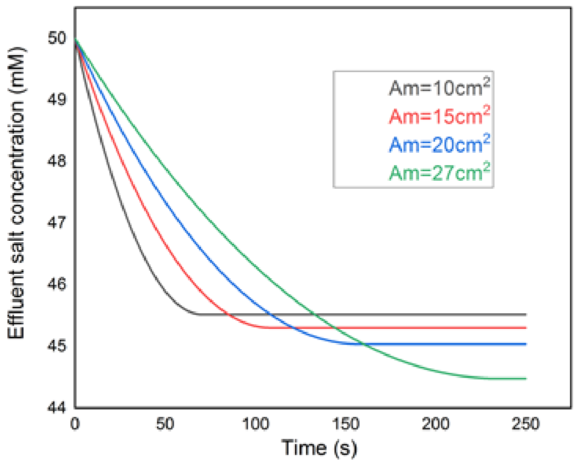

Fig. 3 Diagram of changes in output water concentration over time, when the cross section is variable

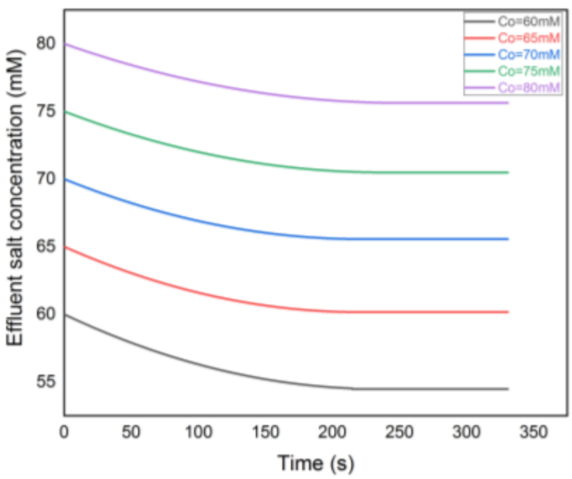

Fig. 4. Diagram of changes in output water concentration over time, when the input concentration is variable

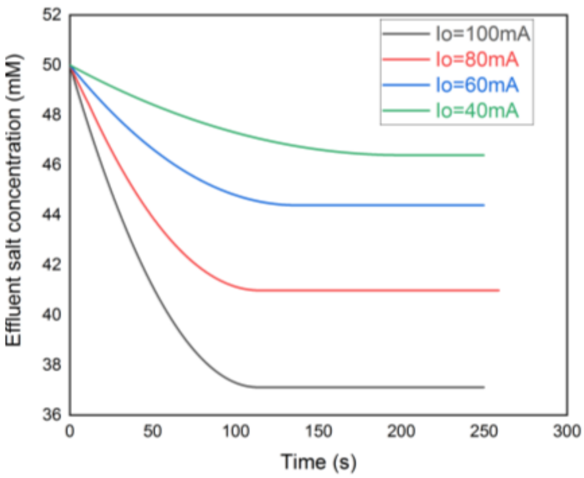

Fig. 5. Diagram of changes in output water concentration over time, when the operating flow of the device is variable

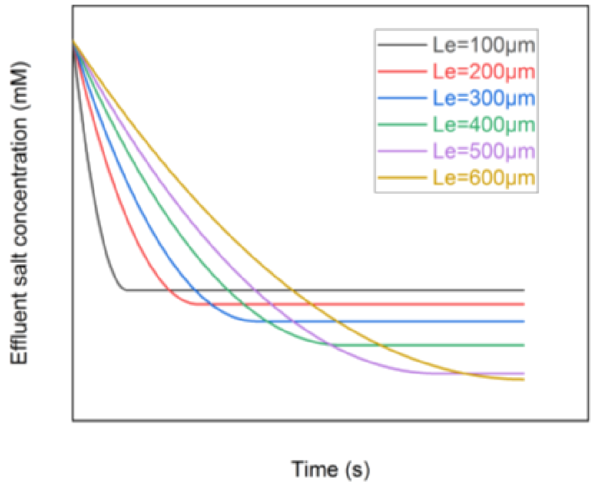

Fig. 6. Diagram of changes in output water concentration over time for different electrode thicknesses

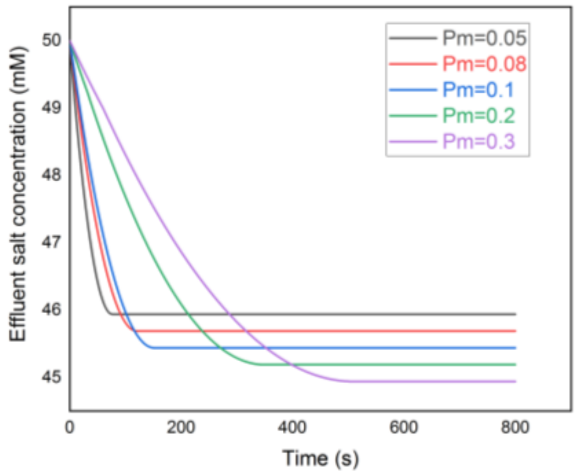

Fig. 7. Diagram of changes in output water concentration over time, when porosity is variable

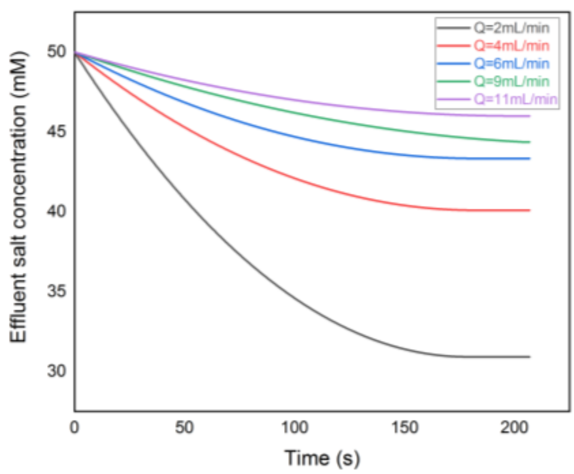

Fig. 8. Diagram of changes in output water concentration over time, when the flow rate is variable

A modeling tool is developed in this paper for the simulation of capacitive deionization systems. The model predicts the efficiency of water desalination and the time required to achieve maximum water desalination. The increase in the efficiency of water desalination and the reduction of time required to achieve maximum water desalination are studied to assess the performance of the device and the optimal operation of the device. The results show that the most effective parameter in improving the Charging current performance by increasing 1.5 times the Charging current flow, the water desalination percentage increased by 72%, and the time required to reach maximum water desalination decreased by 76%.

References

[1] S. Porada, R. Zhao, A. van der Wal, V. Presser, P.M. Biesheuvel, Review on the science and technology of water desalination by capacitive deionization, Progress in Materials Science, 58(8) (2013) 1388-1442.

[2] M. Anderson, A. L. Cudero, J. Palma, Capacitive deionization as an electrochemical means of saving energy and delivering clean water. Comparison to present desalination practices: Will it compete?, Electrochimica Acta, 55 (2010) 3845-3856.

[3] M.E. Suss, T.F. Baumann, W.L. Bourcier, C.M. Spadaccini, K.A. Rose, J.G. Santiago, M. Stadermann, Capacitive desalination with flow-through electrodes, Energy & Environmental Science, 5(11) (2012) 9511-9519.

[4] P.M. Biesheuvel, H.V.M. Hamelers, M.E. Suss, Theory of Water Desalination by Porous Electrodes with Immobile Chemical Charge, Colloids and Interface Science Communications, 9 (2015) 1-5.

[5] Y.A.C. Jande, W.S. Kim, Predicting the lowest effluent concentration in capacitive deionization, Separation and Purification Technology, 115 (2013) 224-230.

[6] Y. Jande, W.-S. Kim, Desalination using capacitive deionization at constant current, Desalination, 329 (2013) 29-34.

[7] Y. Qu, P.G. Campbell, A. Hemmatifar, J.M. Knipe, C.K. Loeb, J.J. Reidy, M.A. Hubert, M. Stadermann, J.G. Santiago, Charging and Transport Dynamics of a Flow-Through Electrode Capacitive Deionization System, The Journal of Physical Chemistry B, 122(1) (2018) 240-249.

HOW TO CITE THIS ARTICLE

A. Abolghasemi, S. Seddighi , Simulation of Effective Parameters on Desalination Water Using Capacitive Deionization Method , Amirkabir J. Mech. Eng., 53(11) (2022) 1401-1404.

DOI: 10.22060/mej.2021.19769.7104