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**ORIGINAL RESEARCH PAPER**

# Parametric Study of Single Pass Mode Capacitive Deionization

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**ABSTRACT:** Due to the ever-increasing human need for potable water, and the limited available resources, various methods of fresh water production have been developed. One of these methods is capacitive deionization which is used in two modes of single pass and batch. In this article, single pass mode capacitive deionization is numerically investigated. A numerical code for simulation the process was developed and validated with some experimental results that are available in the literature. Different effective parameters include applying voltage, feed water flowrate, electrode capacitance, feed concentration and cell volume are considered and their effects on the CDI performance are presented and discussed. Results show that the electrode capacitance is the most important parameter of desalination in CDI technology. Use of electrode with the suitable capacitance can improve the salt adsorption more than 10 times. However, the energy consumption decreases with increasing the cell capacitance up to 2200 F. Further augmentation on the cell capacitance does not have any significant effects on the energy consumption. Therefore, future research should be dedicated to develop the electrodes' electrical and physical properties such as electrode capacitance and its porosity.

**KEYWORDS:** *Capacitive Deionization, Single Pass Mode, Desalination*

## INTRODUCTION

Potable water has been a vital issue for every society for a long time. Due to the limitation of potable water resources, different desalination technology has been developed from various feed sources such as the sea and brackish waters. Most important methods are multi-stage distillation [1], reverse osmosis [2] and forward osmosis [3], electrodialysis [3] and capacitive deionization (CDI) [4–6]. Capacitive deionization, also called electrochemical desalination, is a relatively new method that has received attention in recent decades. Advantages of this method, such as low energy consumption, simplicity of structure, low price, and relatively high efficiency[7], can mentioned compared to other methods. The main mechanism of this method is to place salt ions in the pores of the electrodes. CDI is designed and implemented in single pass [8, 9] and batch modes [10, 11]. The batch mode CDI was simulated and studied in previous work [12]. The overview of single pass mode CDI is shown in Figure 1 [13].

This desalination method was patented by Blair and Murphy in the 1960s [14]. Then a few investigation was conducted to study the CDI system (for instance in the 1970s and 1980s by Oren and Soffer [15, 16] and in the 1990s by Farmer et al. [17]). Recently, due to the increase in water stress problems, researchers' interest in this technology has increased exponentially. In Figure 2, different types of capacitive desalination cell structures are presented. (Figure 2-a) is the same basic structure as mentioned earlier.

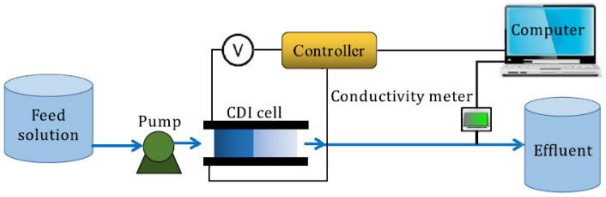



**Fig. 1.** Schematic of single pass mode CDI cell

The next cell structure was developed by Johnson et al. during the 1970s [18, 19], in which the feed flow, parallel to the direction of the applied electric field, was directed through the electrodes (Figure 2-b). This system is called flow-through electrode CDI.

A very important change in the structure of the CDI cell occurred when in 2006, Lee et al. [20] introduced the membrane CDI (MCDI) cell, which involves the use of ion exchange membranes on the separator of each electrode (Figure 2-c). The feed water channels in MCDI cells are surrounded by anion exchange membranes (AEM) at the anode and cation exchange membranes (CEM) at the cathode [21–24]. As researches show, the main advantage of adding membrane to CDI cells is the overall improvement in charge efficiency, because the membranes adsorbs ions of the same sign from the flow and can increase the salt storage in the electrode pores [25, 26]

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**Abbreviations**

| | |
|---|---|
| *AC* | Activated carbon |
| *AEM* | Anion exchange membrane |
| *CDI* | Capacitive deionization |
| *CEM* | Cation exchange membrane |
| *FCDI* | Flow electrode capacitive deionization |
| *GCS* | Gouy-Chapman-Stern model |
| *i-CDI* | Inverted capacitive deionization |
| *MAC* | Modified activated carbon |
| *MCDI* | Membrane capacitive deionization |
| *mD* | Modified Donnan |
| *MSF* | Multi stage flash distillation |
| *NaCl* | Sodium chloride |
| *PWC* | Pooled water concentration |
| *RO* | Reverse osmosis |

**Nomenclature**

| | |
|---|---|
| $c_0$ | Inlet ion concentration $[mM]$ |
| $c_{desorption}$ | Salt concentration at the desorption process $[mM]$ |
| $c_{PW}$ | Pooled water concentration $[ppm]$ |
| $C_{st}$ | Electrode capacitance $[F]$ |
| $c_{effluent}$ | The effluent concentration at the adsorption process $[mM]$ |
| $F$ | Faraday's constant (96485 $[C/mol]$) |
| $M_{NaCl}$ | Molecular weight of NaCl |
| $R_{cell}$ | Resistance of CDI cell $[\Omega]$ |
| $S_{ions}$ | Ion adsorbed in the cell $[g]$ |
| $t_0$ | Initial time $[s]$ |
| $t$ | Time $[s]$ |
| $t_{ad}$ | Adsorption time $[s]$ |
| $V_{cell}$ | Applied voltage $[V]$ |
| $v_{cell}$ | Cell volume $[mL]$ |
| $V_{des}$ | Desorption voltage (for short circuit =0 $[V]$) |
| $v_{sp}$ | Spacer volume $[s]$ |
| $z$ | Ionic valance of inlet water |

**Greek Symbols**

| | |
|---|---|
| $\alpha_i$ | Constant coefficient $[s^{-1}]$ |
| *nf* | $\beta_i$ |
| $\varepsilon$ | Charge efficiency |
| $\phi$ | Volumetric Flowrate $[mL/min]$ |
| $\mu$ | Constant coefficient for adsorption process $[mmol]$ |
| $\mu_{des}$ | Constant coefficient for desorption process $[mmol]$ |

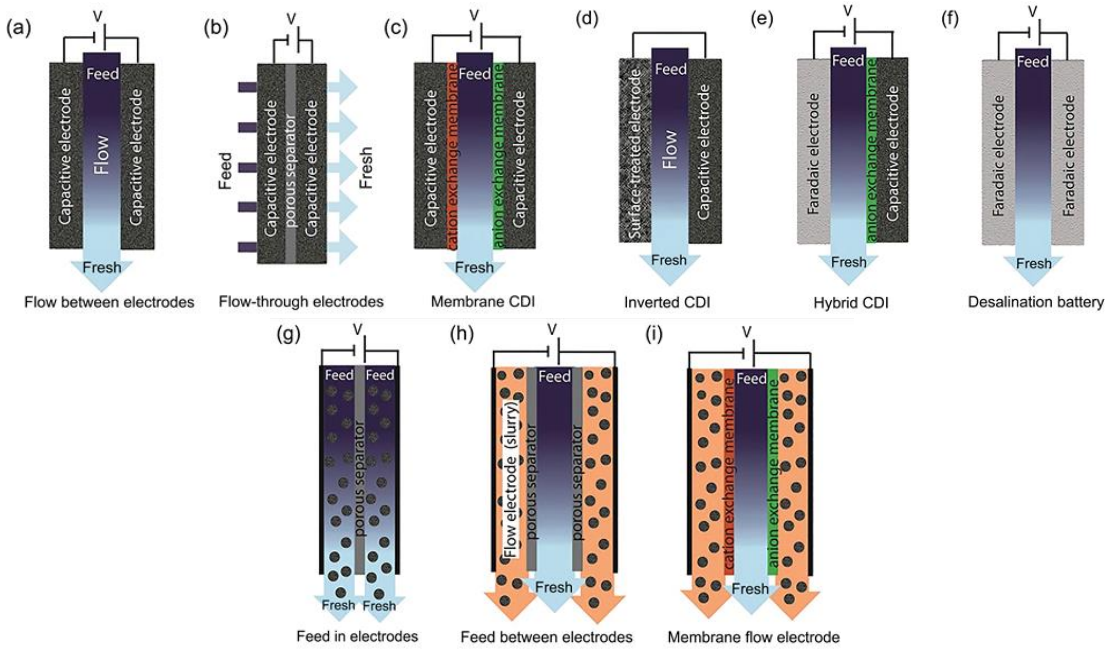



**Fig. 2.** CDI structures using static electrodes (a-f) and current electrodes (g-i) [27]

In past decade, Gao [28] introduced the CDI cell using a surface-modified carbon anode, leading to a new configuration called inverted CDI (i-CDI, Figure 2-d). This cell uses a carbon xerogel electrode with a negative charge on its surface as the anode and a carbon xerogel as the cathode [28, 29]. The reason why it is called "inverted CDI" is that the cell exhibits reverse behavior, meaning that charging the cell leads to the repulsion of ions from the electrical double layers of the electrode, and discharging the cell leads to the electrosorption of ions.

Pasta et al. [30] in 2012 introduced a new structure called "desalination battery" (Figure 2-f), which works similarly to the CDI cell, but instead of ion storage in electrical double layers (in a major part of the electrode material) using

Faradaic processes, storage is done in chemical bonds [31]. The desalination battery they tested consists of a positive $Na_{2-x}Mn_5O_{10}$ nanorod electrode and a negative Ag/AgCl electrode. It was recorded an energy consumption of 0.29 Wh/l for 25% salt removal.

One of the most recent developments in the CDI structure was the presenting of suspended carbon material as flow electrodes in 2013 by Jeon et al. [32]. The concept of flow electrode CDI (FCDI) comes from fluid flow-based electrodes (Figure 2-g to i), which have been developed for electrochemical energy storage systems, such as electrochemical flow capacitors and semi-solid Li-ion batteries [33]. In FCDI, the water flowing through the cell can be desalinated continuously since the discharge of carbon particles in the slurry can occur as a separate process downstream of the cell [32]. It can also solve the complexity of the conventional CDI systems for charge and discharge operations (because the desalination streams and the brine streams passed through the same channel at different times).

Porada et al. [34] proposed a different type of arrangement for the CDI cell, in which the deionization process takes place using a "electrodes in motion". In their work, cell pairs are made of thin wires or rods with the anode wires close to the cathode wires.

Modeling and simulation of the processes related to the CDI have also been done by different researchers. Among them, Ryu et al. [35] simulated a CDI cell using Modelica software by In this study, the influence of the involved parameters in the financial advantages and the performance of the capacitive deionization cell compared to the other methods such as RO and MSF. They showed the competitiveness of CDI compared to other methods in low concentrations.

Rommerskirchen et al. [36] presented a model for a steady-state FCDI cell operating at a constant voltage. The storage of ions in the pores of carbon particles is modeled using the modified Donnan model. The simulations performed with this model are in good agreement with the experimental results and correctly predict the effect of the electrode current on the desalination performance. A combination of adsorption (removal of ions from the solution without potential) and CDI (adsorption of ions due to potential), which were called adsorption-CDI (ACDI) hybrid systems, was developed with a modification of zero charge for activated carbon electrodes by Sufiani et al. [37]. Their modified activated carbon (MAC) electrodes showed a high adsorption capacity compared to the normal activated carbon (AC) electrodes [37].

As seen well understanding of the effect of each process parameters of a CDI technology is crucial for further imporovment. Therefore, the present article aims to numerically explore the effects of different process parameters (applying voltage, feed water flowrate, electrode capacitance, feed concentration and cell volume) of a single pass mode CDI cell on the cell performance including energy consumption and permeate quality of water. The effects of applying voltage, feed water flowrate, electrode capacitance, feed concentration and cell volume on the CDI performance are presented and discussed.

**Problem Definition and Governing Equations**

A simple capacitive deionization cell consists of two electrodes. The electrodes are connected to the current collector and placed at a distance from each other (spacer channel), which is usually filled with a high porosity material (like sponge) as a separator (spacer). The feed water flows between the electrodes. It is schematically shown in Fig. 3.

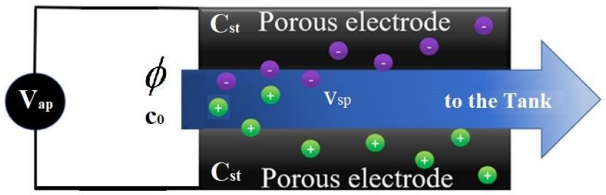



**Fig. 3.** Considered CDI cell

The corresponding equations for presenting the cell mathematical model are as follows. A numerical code is written to solve these equations.

It is assumed that the salt concentration is the same everywhere through the cell. Also, the desalination cell considers to be symmetrical (the anode and the cathode have the same structure). The ion displacement model is based on the modified Donnan (mD) model, but it can also be adjusted based on the GCS[1] model. The model proposed by Jande et al. [38] is developed for the CDI system. During the adsorption process, the effluent concentration ($c_{effluent}$) of the cell is calculated from Eq. (1).

$$c_{effluent}(t) = c_0 - \frac{\mu}{v_{sp}}(e^{-\alpha_1 t} - e^{-\alpha_2 t}) \quad (1)$$

Where $\mu$ ,$\alpha_1$, and $\alpha_2$are constants and are calculated using Eqs. (2)–(4), $c_0$ is the inlet ion concentration, $v_{sp}$ is the total volume of spacer, and $t$ is the desalination time.

$$\mu = \frac{\varepsilon C_{st} V_{ap}}{zF}\left(1 - e^{\frac{\alpha_1 v_{sp}}{\phi}}\right) \quad (2)$$

$$\alpha_1 = 1/R_{cell}C_{st} \quad (3)$$

$$\alpha_2 = \frac{1}{R_{cell}C_{st}} + \frac{\phi}{v_{cell}} \quad (4)$$

In these equations$V_{ap}$is applying voltage, $C_{st}$is the electrode capacitance, $\varepsilon$ is the charge efficiency (≈1), $F$is the Faraday's constant, $z$is ionic valance of inlet water (=1), $R_{cell}$is the cell resistance, $v_{cell}$ is the cell volume, and $\phi$ is the volumetric water flowrate.

1 Gouy-Chapman-Stern

For the desorption process, to remove ions from micropores, reverse voltage or zero voltage is applied to the CDI cell ($V_{des}$). The changes of concentration in the desorption process ($c_{desorption}$) can obtained from Equation 5:

$$c_{desorption}(t) = c_0 - \frac{\mu_{des}}{v_{sp}}(\beta_1 e^{-\alpha_2 t} - \beta_2 e^{-\alpha_1 t}) \quad (5)$$

In this equation$\mu_{des}$,$\beta_1$, and $\beta_2$, are constants and should be calculated from Eq. (6) to Eq.(8).

$$\mu_{des} = \frac{1.3\varepsilon C_{st}\left[V_{ap}(1 - e^{-\alpha_1 t_{ad}}) - V_{des}\right]}{zF}\left(1 - e^{\frac{\alpha_1 v_{sp}}{\phi}}\right) \quad (6)$$

$$\beta_1 = e^{\alpha_2 t_{ad}} \quad (7)$$

$$\beta_2 = e^{\alpha_1 t_{ad}} \quad (8)$$

$V_{des}$ is the discharge cell voltage, and $t_{ad}$is the adsorption time.

Produced water from the adsorption process has been stored in a tank. The average salt concentration of water in the tank for the specific time can be obtained from Eq. (9).

$$c_{PW}(t) = \frac{1}{t_{ad} - t + 1}\left[c_0(t_{ad} - t) + \frac{\mu}{\alpha_1 v_{sp}}(e^{-\alpha_1 t_{ad}} - e^{-\alpha_1 t}) - \frac{\mu}{\alpha_2 v_{sp}}(e^{-\alpha_2 t_{ad}} - e^{-\alpha_2 t})\right] \quad (9)$$

Where $c_{PW}$ is pooled water concentration (PWC). To calculate the quantity of salt molecules adsorbed in desalination process, Eq. (10) is used:

$$S_{ions}(t) = \phi \times M_{NaCl}\int_{t_0}^{t_{ad}}(c_0 - c_{effluent})dt \quad (10)$$

$S_{ions}$is the salt adsorption, and $M_{NaCl}$ is the molecular weight of NaCl.

Finally, the energy consumption of the CDI cell per gram of absorbed salt is obtained from the following equation.

$$E_s = \frac{C_{st}\left[V_{ap}(1 - e^{-\alpha_1 t_{ad}})\right]^2}{2\phi \times M_{NaCl}\left[\frac{\mu}{\alpha_1 v_{sp}}(1 - e^{-\alpha_1 t_{ad}}) - \frac{\mu}{\alpha_2 v_{sp}}(1 - e^{-\alpha_2 t_{ad}})\right]} \quad (11)$$

### Validation

The governing equations of a capacitive deionization cell were presented for a single pass mode cell. Based on these equations and considering a simple symmetrical cell (like Figure 1) a computational code was developed to simulate the considered cell performance. In order to be sure the numerical model can well predict the cell performance comparisons with the experimental results of Zhao et al. [39] and Ryu et al. [35] have been performed. As seen in Figs. 4 and 5 good agreements between the results are seen. Therefore, the mathematical model and numerical procedure is reliable for simulating the cell.

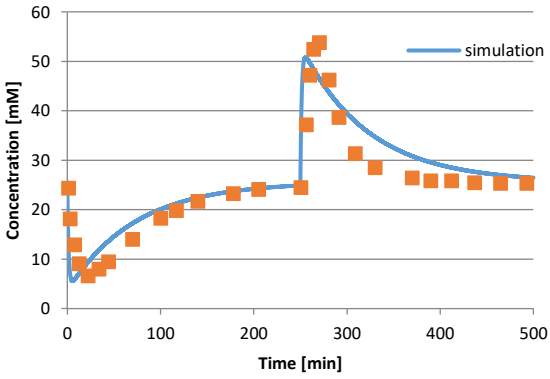



**Fig. 4.** Salt concentration versus time for CDI cell in batch mode, compared to experimental results [35]

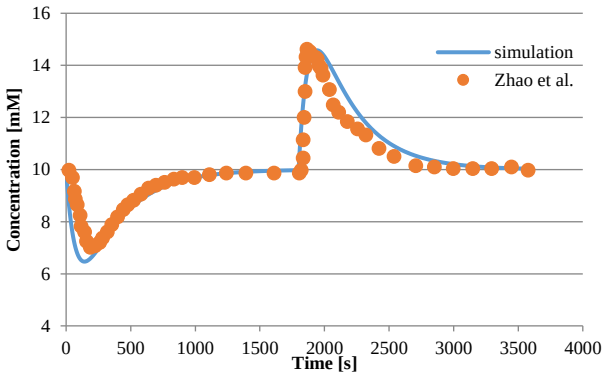



**Fig. 5.** Comparing of the modeled CDI cell with Zhao et al. [39]

## RESULT AND DISCUSSION

Effective parameters on the single pass mode CDI cell listed in Table 1. Variations of these parameters is considered to be in the range of those that can be found in the experimental results of references [35, 39].

**Table 1.** Effective parameters in a single pass mode capacitive deionization cell.

| No. | Parameter | Value | Range |
|---|---|---|---|
| 1 | Applying voltage | $V_{ap} = 1.2\ V$ | 0.8-1.8 |
| 2 | Flowrate | $\phi = 60\ mL/min$ | 30-80 |
| 3 | Electrode capacitance | $C_{st} = 6200\ F$ | 200-10200 |
| 4 | Inlet concentration | $c_0 = 25\ mM$ | 10-35 |
| 5 | Cell volume | $v_{cell} = 100\ mL$ | 60-160 |

According to the Table 1, parameters' effects on salt adsorption, energy consumption, and pooled water concentration is studied. The effect of applying voltage for a given feed water flowrate ($\phi$), cell volume ($v_{cell}$), inlet feed concentration ($c_0$), and electrode capacitance ($C_{st}$) on the

pooled water concentration (PWC), salt adsorption, and the energy consumption are shown in Fig. 6. As seen, increasing the applying voltage, reduces the PWC (about 18 %) and increases the salt adsorption. However, the energy consumption significantly increases (more than 2.25 times) because of increasing the electrical resistance.

Figure 7 shows the effect of feed flowrate on the energy consumption, salt adsorption and PWC. Feed flowrate increasing leads to PWC augments without any notable change in the energy consumption and salt adsorption. It shows that the ion diffusion rate is constant in the spacer volume, so increasing the feed flowrate does not change the salt adsorption and EC.

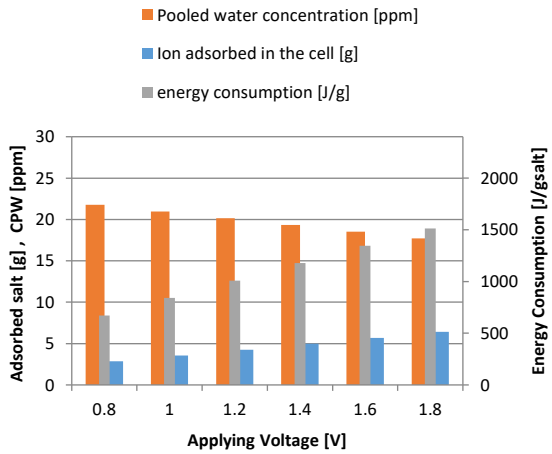



**Fig. 6.** Effect of applying voltage on energy consumption, salt adsorption and pooled water concentration

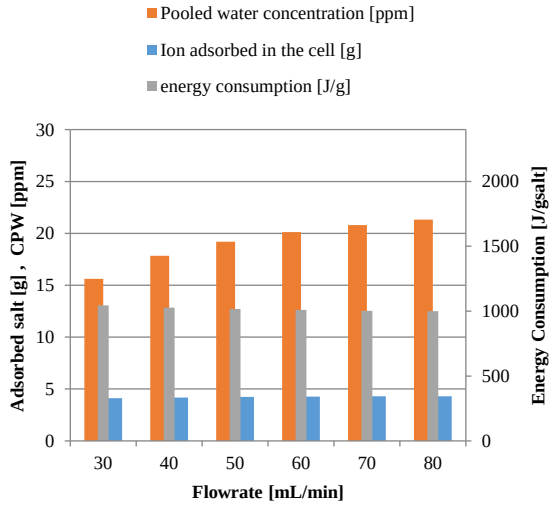



**Fig. 7.** Effect of flowrate on energy consumption, salt adsorption and pooled water concentration

The effect of electrode capacitance for a given cell volume ($v_{cell}$), flowrate ($\phi$), inlet concentration ($c_0$), and applying voltage ($V_{cell}$) on the pooled water concentration (PWC), salt adsorption, and the energy consumption are shown in Fig. 8. As shown, increasing the electrode capacitance results higher salt adsorption, and lower PWC. However, the energy consumption decreases with increasing the cell capacitance up to 2200 F. Further augmentation on the cell capacitance does not have any significant effects on the energy consumption. The result also shows that with the capacitance augmentation, the cell ability for ion adsorption can be enhanced.

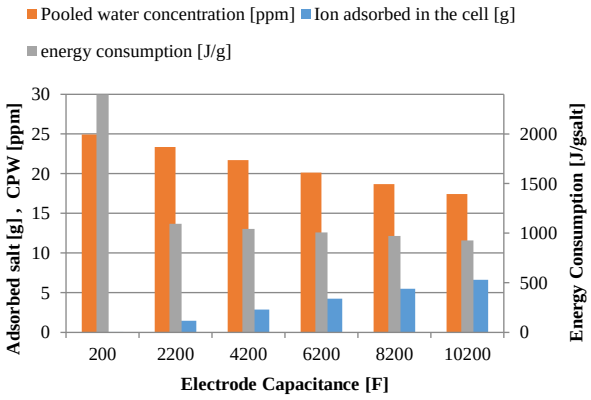



**Fig. 8.** Effect of electrode capacitance on energy consumption, salt adsorption and pooled water concentration

Figure 9 shows the effect of inlet concentration for given cell volume ($v_{cell}$), flowrate ($\phi$), electrode capacitance ($C_{st}$), and applying voltage ($V_{cell}$) on the PWC, salt adsorption, and the energy consumption. The increase of inlet concentration increases the PWC ($c_{PW}$) without any significant change in the energy consumption and salt adsorption. It seems that the cell is saturated and an increase in the inlet concentration augments the PWC.

Figure 10 shows the effect of cell volume on the energy consumption, salt adsorption and pooled water concentration. As seen, $v_{cell}$ does not have any effects on the picked-up functions in this simulation. It seems that the cell is saturated and an increase in the cell volume can't affect the objective functions.

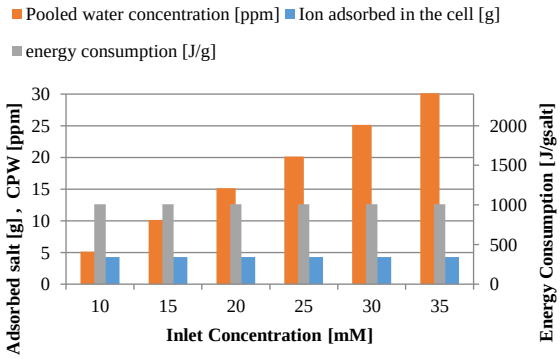



**Fig. 9.** Effect of inlet concentration on energy consumption, salt adsorption and pooled water concentration

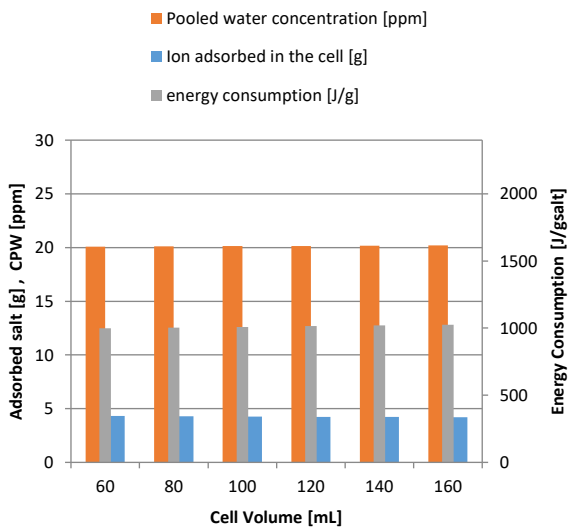



**Fig. 10.** Effect of cell volume on energy consumption, salt adsorption and pooled water concentration

## CONCLUSION

In this paper a single pass mode capacitive deionization cell for desalination water is numerically investigated using a home-made reliable numerical code. The effects of variations of applying voltage, feed water flowrate, electrode capacitance, feed concentration and cell volume are on the CDI performance are investigated. The result shows that the electrode improvement can improve the CDI performance and with the capacitance augmentation, the cell ability for ion adsorption can be enhanced. It is found that the ion diffusion rate is constant in the spacer volume, so increasing the feed flowrate does not change the salt adsorption and energy consumption. Based on the resent result and our previous finding [12] the electrode electrical and physical properties are the most important parameters for improving the cell performance. Results show that the electrode capacitance is the most important parameter of desalination in CDI technology. The capacitance can be improved by adding the negative and positive functionalized group to the electrodes. Therefore, future research should be dedicated to develop the electrodes' electrical and physical properties such as electrode capacitance and its porosity.

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**Conflict of Interest**

The authors have declared no conflict of interest.

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